Report No. FAA-RD-71-111,3

AD 741570

THE CONTROL OF OXIDES AND NITROGEN EMISSIONS FROM AIRCRAFT GAS TURBINE ENGINES

Volume 3: The Flow Model

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transpo 72
U.S. International Transportation Exposition
Dulles International Airport
Washington, D.C.
May 27–June 4, 1972

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DECEMBER 1971
FINAL REPORT

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DEPARTMENT OF TRANSPORTATION
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Systems Research & Development Service
Washington, D.C. 20591

ENVIRONMENTAL PROTECTION AGENCY
Office of Air Programs
ANN ARBOR, MICH. 48105

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173

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A

TECHNICAL REPORT STANDARD TITLE PAGE

1. Report No.	2. Government Accession No.	3. Recipient's Catalog No.
FAA-RD-71-111-3		

4. Title and Subtitle

THE CONTROL OF OXIDES OF NITROGEN EMISSIONS FROM AIRCRAFT GAS TURBINE ENGINES
VOLUME 3: THE FLOW MODEL

5. Report Date

December, 1971

6. Performing Organization Code

7. Author(s)

Ronald S. Fletcher
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8. Performing Organization Report No.

1162-3

9. Performing Organization Name and Address

Northern Research and Engineering Corporation
219 Vassar Street
Cambridge, Massachusetts 02139

10. Work Unit No.

11. Contract or Grant No.

DOT FA70WA-2428

12. Sponsoring Agency Name and Address

Department of Transportation
Federal Aviation Administration
Washington, D. C. 20590

Environmental Protection Agency
Office of Air Programs
Ann Arbor, Michigan 48105

13. Type of Report and Period Covered

Final Report:
June, 1970-December, 1971

14. Sponsoring Agency Code

15. Supplementary Notes

16. Abstract

The objective of this study was to develop criteria for use in the design of aircraft gas turbine combustion chambers to minimize nitrogen oxide emissions. The approach adopted involved the development of a mathematical model of NOx emission from aircraft engine combustors; a parametric analysis, using the model, to determine the sensitivity of NOx emissions to variations of model parameters and engine design variables; evaluation of critical model parameters by means of experimental measurements; and the incorporation of the model into combustor design methods to provide guidelines for minimizing NOx emission while maintaining other performance and emission characteristics. The results of the study and the NOx emission control criteria are described in Volume 1 (FAA-RD-71-111-1). Volume 2 (FAA-RD-71-111-2) describes the nitric oxide formation process and a computer program (NOXRAT) for calculating thermodynamic data. The program is based upon a six-reaction model of NO formation. Volume 3 (FAA-RD-71-111-3) describes combustion and flow processes in gas turbine combustors and a computer program (GASNOX) for calculating gas properties and NO concentrations throughout a combustor. This program is based upon a three-zone, heterogeneous model of gas turbine combustor operation. Program GASNOX is used with input data from Program NOXRAT to calculate NO emission rates.

17. Key Words

Air Pollution, Nitrogen Oxides, Nitric Oxide, Aircraft, Gas Turbine, Theoretical Model, Experimental Measurement, Design Criteria

18. Distribution Statement

Availability is unlimited. Document may be released to the National Technical Information Service, Springfield, Virginia 22151, for sale to the public.

19. Security Classif. (of this report)	20. Security Classif. (of this page)	21. No. of Pages	22. Price
UNCLASSIFIED	UNCLASSIFIED	173	$3.00 PC .95 MF

Form DOT F 1700.7 (8-69)

The study reported here was carried out under the technical direction of Dr. D. M. Dix with Dr. Ronald S. Fletcher assuming project responsibilities. Other participants in the program were Dr. R. D. Siegel, Dr. E. K. Bastress, and Mr. R. J. Murad; Professors J. B. Heywood, A. H. Lefebvre, and Mr. E. R. Norster served in a consulting capacity during the course of the study.

This study was sponsored in part by the Federal Aviation Administration and the Environmental Protection Agency under Contract No. DOT FA70WA-2428. Technical monitoring of the program was conducted by Mr. William T. Westfield (FAA) and Mr. George D. Kittredge (EPA).

CONTENTS

CONTENTS (CONTINUED)

LIST OF FIGURES

1. INTRODUCTION

Volume 1 of this report carries a full description of the complete program but omits mathematical details of the model developed to predict the nitric oxide (NOx) emissions from aircraft gas turbine combustors and also the details of two computer programs developed as part of the study for obtaining predictions from the model. It is the purpose of Volumes 2 and 3 of the report to present full descriptions of both the model and the computer programs.

It is convenient to consider the model in two parts, one part being concerned with the NOx formation process and the other with modeling the flow behavior within gas turbine combustors. The convenience arises not only due to the basic difference in the studies of these two parts, but also due to the fact that a separate computer program has been developed for each part. This approach has been adopted in the interests of economy of computation as calculation of the necessary data for the determination of the NOx formation process requires appreciable computer time but the data once collected can, of course, be applied to any combustion calculation with the same reference conditions (in this case, combustor inlet conditions) of pressure and temperature. The computer program developed for this task has the name NOXRAT, and its function is to compute the rate terms of the NOx formation process and all relevant thermodynamic data for a series of fuel-to-air ratios with a common reference state.

Volume 2 of this report is solely concerned with the nitric oxide formation process. It presents a mathematical description of the program NOXRAT and also includes a section which is essentially a user's manual for the program. Volume 3 produces the same details for the flow model developed to describe the flow conditions in a gas turbine combustor. The corresponding computer program is named GASNOX and it is so arranged that the rate terms and all relevant thermodynamic data computed in NOXRAT are punched onto a deck of computer cards which serves as input data to the main program GASNOX.

The objective of this volume of the report, therefore, is to present the theory behind the flow model and details of the computer program developed for its application.

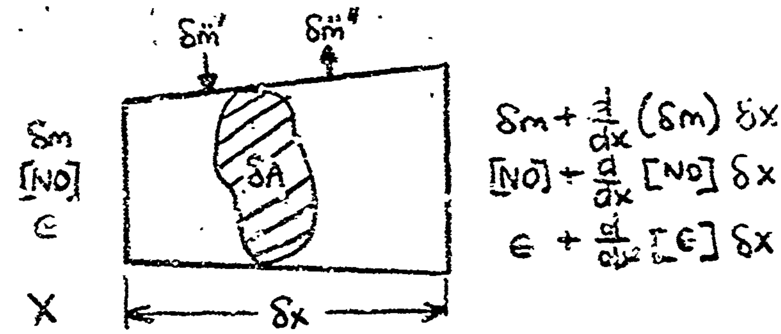
2. THE FLOW MODEL

Calculations based upon the reaction scheme described in Volume 2 clearly show that for significant concentrations of nitric oxide to be formed during the short time it takes the gases to pass through an aircraft gas turbine engine, the temperature must exceed 2000 deg K. Such high temperatures only exist within the combustor, and only then for a limited time, so clearly, nitric oxide concentrations in the exhausts of aircraft engines are solely dependent upon the flow behavior and the chemical processes occurring within the combustion chamber and it is these features that must be adequately represented in the model.

The first task, therefore, is to select a method of modeling the flow processes in the gas turbine combustor. Such combustors are conventionally divided into three zones as shown in Figure 1a. The distinction between these zones is discussed qualitatively in Volume 1, Section 3, but in the next section these distinctions are quantified. Firstly, the basic conservation equations are derived for the generalized case of an inhomogeneous, reacting gas mixture of the type that occurs in a gas turbine combustor. These equations are then reduced to conditions applicable to the three combustor zones, the primary, intermediate and dilution zones, which are of interest to this study, and finally, they are used to demonstrate how the nitric oxide levels may be calculated for each zone.

2.1 THE GENERALIZED CONSERVATION EQUATIONS

A control volume will be considered to contain products of constant fuel-to-total mass ratio, $\mathcal{F}$, which will be termed the mixture ratio. (The constancy of $\mathcal{F}$ is taken as it has particular utility in this study insofar as that it minimizes the number of calculations for the equilibrium conditions necessary to determine local nitric oxide reaction rates.) The volume is as shown below:



where, δm = mass flow in interval δF about F

$[NO]$ = mass fraction of nitric oxide

ϵ = m_{fu}/m, fractional mass flow of unburned fuel

$\delta\ddot m'$ = mass flow per unit length of fuel ratio F', with mass fraction of NO = $[NO]'$ which enters the volume due to mixing

$\delta\ddot m''$ = mass flow per unit length, with mass fraction of NO = $[NO]''$ which leaves the volume due to mixing

δA = cross sectional area of element

$\dot r$ = rate of formation of NO per unit volume by chemical reaction

The conservation equations become,

for NO, $$\frac{d}{dx}\left(\delta m[NO]\right) = \dot r\,\delta A + \delta\ddot m'[NO]' - \delta\ddot m''[NO]'' \qquad \text{A-1}$$

mass, $$\frac{d}{dx}(\delta m) = \delta\ddot m' - \delta\ddot m'' - \frac{d}{dx}(\epsilon\,\delta m) \qquad \text{A-2}$$

burned fuel, $$F\frac{d}{dx}(\delta m) = \delta\ddot m' F' - \delta\ddot m'' F'' - \frac{d}{dx}(\epsilon\,\delta m) \qquad \text{A-3}$$

unburned fuel, $$\frac{d}{dx}(\epsilon\,\delta m) = \dot R \quad \text{- specified} \qquad \text{A-4}$$

In the limit as dX tends to zero, these equations take the form,

$$\frac{d}{dx}\left([NO]\frac{dm}{dF}\right) = \dot r\frac{dA}{dF} + [NO]'\frac{d\ddot m'}{dF} - [NO]''\frac{d\ddot m''}{dF} \qquad \text{A-1a}$$

$$\frac{d}{dx}\left(\frac{dm}{dF}\right) = \frac{d\ddot m'}{dF} - \frac{d\ddot m''}{dF} - \frac{d}{dx}\left(\epsilon\frac{dm}{dF}\right) \qquad \text{A-2a}$$

$$F\frac{d}{dx}\left(\frac{dm}{dF}\right) = F'\frac{d\ddot{m}'}{dF} - F''\frac{d\ddot{m}''}{dF} - \frac{d}{dx}\left(\epsilon\frac{dm}{dF}\right) \qquad \text{A-3a}$$

$$\frac{d}{dx}\left(\epsilon\frac{dm}{dF}\right) = \dot{R} \qquad \text{A-4a}$$

2.2 THE DISTRIBUTION FUNCTION

The control volume considered above is only concerned with an element of mass δm with a mixture ratio δF about F. It was proposed to represent the distribution of mass about mixture ratio by a normal distribution function of the form,

$$\frac{\delta m}{\delta F} = C\exp\left\{-\frac{1}{2}\left(\frac{F-\bar{F}}{\sigma}\right)^2\right\} \qquad \text{A-5}$$

The parameter σ, in statistical terms, is called the standard deviation and represents the degree of distribution of F about the mean value $\bar{F}$. C is termed the normalizing factor and for the purpose of this study is defined by the expression that,

$$\int_0^{2\bar{F}} \frac{\delta m}{\delta F}\cdot dF = \dot{m}(1-\epsilon) \qquad \text{A-6}$$

The value of $\bar{F}$ is the ratio of the total fuel burned to the total mass flow. Clearly both C and $\bar{F}$ will be a function of the axial position in the combustor as they are computed from Equations A-2 and A-3.

A normal distribution has been selected as it is known to fit the spray characteristics of the type of fuel injectors used in gas turbine combustors and it provides a convenient way of describing the mixing process, by specification of the relationship $\sigma = \sigma(x)$. The value of δm_i, the mass flow in interval δF about F_i can also be evaluated functionally by the equation form,

$$\delta m_i = \int_{F_i-\delta F/2}^{F_i+\delta F/2} \delta m/\delta F \; dF \qquad \text{A-7}$$

and so the whole flow field can be readily represented by a series of discrete elements of constant, but different, mixture ratios.*

2.3 APPLICATION TO THE PRIMARY ZONE

The model of the flow behavior described previously assumes that no mixing takes place in the primary zone after the specified distribution of mass mixtures ratios is attained. Thus, referring to the control volume above,

$$\delta \dddot{m}' = \delta \dddot{m}'' = 0$$

and further, it is also assumed that only a certain fraction β of the total fuel entering the zone is burned and that this fraction burns instantaneously.

$$\frac{d}{dx}\left(\epsilon\, \delta m\right) = 0$$

so equation (A-1) reduces to,

$$\frac{d}{dx}\left(\delta m\,[NO]\right) = \dot{r}\,\delta A \qquad \text{A-8}$$

or,

$$[NO]_x = \int_0^x \frac{\dot{r}\,\delta A}{\delta m}\,dx \qquad \text{A-9}$$

or alternatively.

$$[NO]_t = \frac{1}{\rho}\int_0^t \dot{r}\,dt \qquad \text{A-10}$$

where ρ is the density of the element and t is the time it takes to pass through the primary zone. It is taken that $\rho = \bar{\rho}$, the mean density in the primary zone where,

$$\bar{\rho} = \frac{1}{\dot{m}}\int_0^{2\bar{F}} \rho \cdot \frac{\delta m}{\delta F}\,dF \qquad \text{A-11}$$

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* The nature of the normal distribution function is that f(F)dF only tends to zero as F tends to $\pm\infty$. Negative F's have no physical significance so a constraint is imposed upon the function that $0 < F < 2\bar{F}$ thus preserving the useful feature of symmetry about $\bar{F}$. In fact, if σ is less than $\bar{F}/3$, this constraint modifies the function to only a very small extent as it can be shown that the integral is greater than 99.7 per cent of that over the range $\pm\infty$. Practically, a range of σ from 0 to $\bar{F}/3$ will represent a wide range in distribution characteristics. It should also be noted that C and m are simply related by the equation $C = \sqrt{2\pi}\,\sigma m$, if the limits are expressed from $\pm\infty$.

but the value of t cannot be so simply expressed for the case of a completely-stirred reactor. Theoretical considerations dictate (see Ref 1) that various fractions of the mass flow δm have different residence times according to the function,

$$F(t) = \frac{1}{\bar{\tau}} \exp(-t/\bar{\tau}) \qquad \text{A-12}$$

where $\bar{\tau}$ is the mean residence time and is equal to the ratio of $(V_P\bar{\rho}/\dot{m})$ and where V_P is the volume of the primary zone. The relationship,

$$f(t) = F(t)dt = \frac{1}{\bar{\tau}} \int_{t-\frac{1}{2}dt}^{t+\frac{1}{2}dt} \exp(-t/\bar{\tau})\,dt \qquad \text{A-13}$$

then defines a fraction f_t of δm which has a residence time within the range dt about t. It is therefore necessary to solve Equations A-10 and A-13 to compute a series of f_t values corresponding to the $[NO]_t$ concentrations over the range of t from zero to infinity. The mean nitric oxide concentration at the exit of the zone for an element of mixture ratio F, $[\overline{NO}]_F$, is then calculated from,

$$[\overline{NO}]_F = \sum_{t=0}^{t=\infty} f_t \times [NO]_t \qquad \text{A-14}$$

and the process repeated for all elements over the mixture range of interest.

Finally, an over-all mass mean average nitric oxide concentration for all products leaving the primary zone can then be computed by summing all products $[\overline{NO}]_F \times \delta m$ and dividing by the total mass flow rate through the primary zone.

2.4 APPLICATION TO THE INTERMEDIATE ZONE

In the intermediate zone, mixing is assumed to occur over the length of the zone L, such that at the exit it is uniformly mixed. We postulate that mixing is characterized by the expression,

$$\sigma = \sigma_o \left\{1 - \left(X_I/L\right)^{A_1}\right\} \qquad \text{A-15}$$

where σ_o is the prescribed deviation for the primary zone, A_1 is a model constant and X_1 is the axial distance from the primary zone exit. The distribution of the mixture ratio F is therefore known at every point, i.e., $\delta m = f(F, X)\, \delta x$ is prescribed by Equations A-5, A-6, and A-15. The problem therefore reduces to determining $\delta \ddot{m}'$, $\delta \ddot{m}''$, and F' from Equations A-2 and A-4 and to making certain assumptions about the mixing process, as $[NO]'$ and $[NO]''$ must be determined in order that Equation A-1 can be solved for $[NO]$ as a function of F and X.

We will postulate that all mixing occurs at conditions corresponding to entry conditions into the control volume so,

$$[NO]'' = [NO]$$

$$[F]'' = F$$

and also that,

$$\delta \ddot{m}'' = K \delta m \qquad \text{A-16}$$

which is to say that the flow out of the elemental control volume, due to mixing, is proportional to the amount flowing into the control volume. Clearly K must have units of 1/length and the physical interpretation of K can best be thought of in terms of the ratio, C_N, of the mass flow rate leaving the element over the length of the intermediate zone to the mass flow rate within the element. If this latter mass flow rate is constant, then clearly

$$\delta \ddot{m}'' = C_N \delta m$$

or,

$$K = C_N / X_L$$

It will be assumed that the value of K is known. Equation A-2 then yields,

$$\delta \ddot{m}' = \frac{d}{dx}(\delta m) + \dot{R} + K \delta m \qquad \text{A-17}$$

where it is to be noted that the restrictions,

$$K > 0$$
$$K > \left\{ -\frac{1}{\delta m}\left(\frac{d}{dx}(\delta m) + \dot{R}\right)\right\}_{max} \qquad \text{A-18}$$

must be satisfied for the model to be valid.

The gases flowing into the control volume as a result of mixing, $\delta\ddot{m}'$, will originate from two sources: firstly, from the mixing of gases already within the combustor liner, which we will denote as $\delta\ddot{m}_m$ and secondly by the mixing action of the diluent air with previously mixed gases, which we will call $\delta\ddot{m}_a$. Clearly,

$$\delta\ddot{m}' = \delta\ddot{m}_m + \delta\ddot{m}_a \qquad \text{A-19}$$

and we will postulate that,

$$\delta\ddot{m}_a = \frac{\delta m}{m}\ddot{m}_a \qquad \text{A-20}$$

that is, that the amount of diluent air entering the control volume is in proportion to the total mass flow rate in the volume. The problem is then defined in terms of $\delta\ddot{m}'$, $\delta\ddot{m}''$, and F' as,

$$\delta\ddot{m}_m = \frac{d}{dx}(\delta m) + K\delta m - \frac{\delta m}{m}\dot{m}_a + \dot{R} \qquad \text{A-21}$$

from Equations A-17, A-19, and A-20, and also as a consequence of Equation A-3.

$$F' = \frac{F}{\delta\ddot{m}'}\left(\delta\ddot{m}'' + \frac{d}{dx}(\delta m)\right) + \frac{\dot{R}}{\delta\ddot{m}'} \qquad \text{A-22}$$

The value of [NO] must now be calculated. Clearly, the total nitric oxide mass which leaves all the elements by mixing must also return via the mixing process to preserve conservation of the specie. The following relationship is assumed to apply, therefore, that

$$[NO'] \sum_{0}^{2\bar{F}} \delta\ddot{m}' = \sum_{0}^{2\bar{F}} \left(\delta\ddot{m}'' \times [NO]''\right) \qquad \text{A-23}$$

The value of $\dot{R}$, the rate of burning of the unburned fuel which leaves the primary zone (see Equation A-4), is now all that is necessary to calculate NO concentrations throughout the intermediate zone.

It is postulated that this rate of burning is controlled by the mixing process, so in keeping with the Equation A-15, the following is assumed,

$$\varepsilon = \varepsilon_o \left(1 - A_3 \left(x_I/L\right)^{A_2}\right) \qquad \text{A-24}$$

where A_2 and A_3 are model constants, ε_o is the fractional mass of unburned fuel entering the intermediate zone and is given by*,

$$\varepsilon_o = (1-\delta)\, \dot{m}_F/\dot{m} \qquad \text{A-25}$$

$\dot{R}$ may therefore be computed, as by definition (see Equation A-4), it is equal to $\frac{d}{dx}(\varepsilon \delta m)$. Thus the problem is defined as,

$\delta \ddot{m}'$ is known from Equations A-19 and A-21

$\delta \ddot{m}^*$ is known from Equation A-16

$[NO]'$ is known from Equation A-23

$[NO]''$ is equal to $[NO]_x$

and $\delta m = F(F,x)\delta F$, is given by the specified distribution function.

If these values are substituted into the conservation equation for nitric oxide (Equation A-2) then it can be shown that,

$$[NO]_{x+dx} - [NO]_x = \int_x^{x+dx} \frac{\dot{r}}{\rho V}\, dx + \int_x^{x+dx} [\Delta NO] K\, dx$$

$$+ \int_{\delta m}^{\delta m + d\delta m} \left([\Delta NO] + \varepsilon [NO']\right) \frac{d\delta m}{\delta m} + \int_{\varepsilon}^{\varepsilon + d\varepsilon} [NO]' d\varepsilon \qquad \text{A-26}$$

where V is the velocity and,

$$[\Delta NO] = \left([NO]' - [NO]_x\right) \qquad \text{A-27}$$

This equation has to be evaluated in a stepwise manner in order to calculate the relationship $[NO] = F(F,x)\,\delta x$ in the intermediate zone. It is then a simple matter to compute an over-all mass average nitric oxide concentration at each axial station from,

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* Another way to express these relationships is as:

$$\dot{m}_{fu_o} = (1-\delta)\, \dot{m}_f$$

$$\dot{m}_{fu} = \dot{m}_{fu_o}\left(1 - A_3 (x_I/L)^{A_2}\right)$$

$$[NO]_x = \frac{1}{\dot{m}} \sum_{F=0}^{F=2\bar{F}} [NO]_{F,x}\, \delta m \qquad \text{A-28}$$

and so complete the computation.

2.5 APPLICATION TO THE DILUTION ZONE

In the dilution zone all gases are assumed to perfectly mix to a mean mixture ratio. All fuel is assumed to have been burned previously in the combustor and only diluent air enters the zone. For this case therefore, one cannot consider a control volume of constant mixture ratio F, as was done at the introduction to this section, as F must change with axial distance due to the added air flow. For the special case of the assumptions made above, this change may be accounted for by modifying only Equation A-3 of the conservation equations so that this dependency of F with X is properly accounted for.

The conservation Equations A-1 through A-4, can be shown to be given by,

$$\frac{d}{dx}(\delta m [NO]) = \dot{r}\, \delta A$$

$$\frac{d}{dx}(\delta m) = \delta \ddot{m}_a$$

$$\frac{d}{dx}(\delta m F) = 0$$

$$\frac{d}{dx}(\varepsilon\, \delta m) = 0$$

as the above assumptions imply that,

$$\delta \dot{m}'' = \delta \ddot{m}_a$$

and,

$$[NO]' = F' = \dot{R} = \delta \dot{m}'' = 0$$

The conservation equation for nitric oxide can be reduced to the form,

$$[NO]_{x+dx} - [NO]_x = \int_x^{x+dx} \frac{\dot{r}}{\rho V}\, dx + \int_F^{F+dF} \frac{[NO]}{F}\, dF \qquad \text{A-29}$$

which predicts directly, the mean average nitric oxide concentration at the new axial position. This process can be repeated in a stepwise manner to the end of the combustion chamber and hence the nitric oxide concentration at the exit plane may be predicted.

2.6 COMPUTATIONAL PROCEDURE

A summary is presented below of the computational procedure necessary to combine the flow model and the chemical reaction scheme presented in Volume 2 in order to predict nitric oxide emissions from aircraft turbine engines.

2.6.1 Required Input

The following input is required in order for the computation to proceed:

a. Chemical Reaction Scheme

1. A means of evaluating the adiabatic flame temperature, density and composition of the equilibrium products for the combustion of hydrocarbons in air. Program NOXRAT described in Volume 2 serves the purpose.
2. Values of the rate constants k_1 to k_i.
3. Fuel properties in terms of C:H ratio.

b. Combustor Dimensions

These should be expressed in such a way as to allow calculation of,

1. Volume of the primary zone.
2. Area of the intermediate and dilution zones as a function of distance x.

c. Combustor Operating Conditions

The following should be expressed as a function of aircraft operating mode,

1. Combustor inlet temperature and pressure.
2. Total fuel flow rate.
3. Air-flow conditions in terms of the fraction entering the primary zone and the rate of addition at the walls as as it varies with axial position along the combustor.

d. Other Inputs to be Specified

1. The functions,

$\sigma = \sigma(x)$ (see Equation A-15)

and, $\epsilon = \epsilon(x)$ (see Equation A-24)

2. The value of K, or C_N, which defines the fraction of gases that leave an element of constant mixture ratio F due to mixing (see Equation A-16)

2.6.2 Preliminary Calculations

Two preliminary calculations must be performed before the computation of NO concentration levels can be undertaken.

These involve,

a. The determination of a value for β, the fraction of total fuel entering the primary zone that is burned in the zone.

b. A consideration of the mixing characteristics of the cooling air that enters the combustor liner from the walls of the intermediate and dilution zones. The bulk of such flow normally enters perpendicular to the direction of the mainstream product flow and has then to be deflected and entrained before it can enter the fully developed mixing processes. This action must require a finite time (i.e., distance) to occur, and its effect upon the nitric oxide formation process has to be considered.

Combustion Efficiency

A correlation does exist to relate primary zone combustor efficiency to the fuel loading parameter $\dot{m}_f/V_p P^2$. The correlation is given in Reference 2 and is reproduced in Figure 2. There is significant scatter in the data points used to obtain the correlation and the values of the primary zone efficiency determined using the correlation can be expected to have error limits of approximately $\pm$ 20 per cent of the indicated value.

Air Distribution Characteristics

In the calculation of the rate of diluent air addition to the intermediate and dilution zones, some provision must be made for the time (hence distance) necessary for the dilution gases to mix into the mainstream flow. This mixing lag could conceivably affect NO

emissions significantly under certain circumstances as it controls the rate of temperature change at positions downstream of the primary zone exit. A simple method was developed to take some account of this effect and is described fully in Appendix XVI. The method is consistent with the mixing assumptions used to develop the model for the intermediate zone of the combustor and at the same time, it determines the fraction of the air that enters the primary zone.

2.6.3 Prediction Procedure

In the interests of economy of use of Program NOXRAT which determines the flame temperatures and concentrations of the C-H-O-N species at equilibrium conditions, hence the NO formation rates, the distribution function of mixture ratio F, versus mass fraction (Equation A-5), is considered as a series of elements of differing δF. The first task in each step is to calculate the mass fraction in each element from the equation,

$$dm = \int_{F-\delta F/2}^{F+\delta F/2} \delta m/\delta F \, dF$$

for the prescribed conditions and thus relate δm to F.

The δF increments are selected, then the adiabatic flame temperatures T, the density ρ and the corresponding equilibrium concentrations of the species N, N_2O, NO, C_2, O, OH, and NO are determined from Program NOXRAT for each F. These specie concentrations are then used to determine the values of R_1, R_6, K_1, and K_2 (for each F) which are needed to compute the rate of nitric oxide formed by chemical reaction and the calculation then proceeds as follows.

Primary Zone

a. The specified value of β, the fraction of fuel burned in the primary zone, is used to compute $\bar{F}_p$. δm can then be determined for all F values over the range of interest $(0 < F < 2\bar{F}_p)$.

b. The value of the mean residence time $\bar{\tau}$ is determined from Equation A-12.

c. Nitric oxide concentrations at the primary zone exit can then be computed for each F and for the prescribed residence time distribution by solving in an iterative manner the relationship,

$$[\bar{NO}]_F = \sum_{t=0}^{t=\infty} [NO]_t \times f_t$$

d. Finally the mass average nitric oxide concentration is computed for all gases leaving the primary zone from the relationship,

$$[\bar{NO}]_p = \sum_{F=0}^{F=2\bar{F}} [NO]_F \times \delta \dot{m}$$

Intermediate Zone

The calculation procedure for this zone, for each incremental step in the axial direction, is essentially identical to that for the primary, except for the necessity to compute a change in NO concentration due to the mixing process. The procedure is as follows:

a. For $X = X + dX$, new values of $\delta \dot{m}$ are computed at each F from Equation A-5.

b. The value of $[NO]'$, the concentration of nitric oxide in the gases entering the control volume by mixing over the step is computed according to Equation A-23.

c. The nitric oxide concentration at position $X + dX$ is then computed for each mixture ratio F by integration of Equation A-26.

d. Finally the new mass average nitric oxide concentration is computed as for Step d above.

These steps are repeated to the end of the intermediate zone.

Dilution Zone

The results of the intermediate zone calculation serve as input to the dilution zone. At this stage all elements in the combustor are

of equal composition and temperature, and dilution proceeds by the addition of pure air and so one can use the relationship (see Equation A-29) that,

$$[NO]_{x+dx} - [NO]_x = \int_x^{x+dx} \frac{\dot{r}}{\rho V} dx + \int_F^{F+dF} \frac{[NO]}{F} dF$$

This can be integrated in a stepwise manner with respect to X by interpolation of the nitric oxide rate data at each step to determine the nitric oxide concentration conditions at the corresponding F value.

The nitric oxide formation rate quickly reduces in this zone as the temperature decreases rapidly.

3. PROGRAM GASNOX

3.1 INTRODUCTION

3.1.1 Program Function and Capabilities

Program GASNOX is a digital computer program written in Fortran IV language for use with the CDC 6600 computing system. The program has been developed for the purpose of predicting the nitric oxide emission level from an aircraft gas turbine combustor. Based on a given set of combustor dimensions, operating conditions, kinetic rate constants, thermodynamic properties, equilibrium compositions, and a primary zone mixing parameter, the program will compute nitric oxide concentrations as a function of axial position in annular and cananular combustors.

The analytical procedures on which the computer program is based have been discussed in Section 2 of this volume and in Reference 3. Briefly the model considers a combustor to consist of three zones: primar intermediate, and dilution. The primary zone is modeled as a partially stirred reactor with the variation of gas composition, temperature, and residence time occurring within the zone taken into account statistically. The program predicts only the gross features of the flow at the zone exit. The intermediate zone represents a transition between the primary and dilution zones. Here mixing occurs between the heterogeneous products from the primary zone and the entering cooling air. The program predicts the gross features of the flow as a function of axial position in this zone. In the dilution zone, the flow is uni-dimensional with the gases uniformly mixed across each cross section. Only the mean mixture ratio is considered, and this only changes as the remaining compressor air is mixed into the combustor. The procedures incorporated into the program have been found to be quite acceptable in terms of accuracy and calculation efficiency.

3.1.2 Report Arrangement

The main body of the report begins with a section in which the input data necessary for the solution of any case are described in detail; this includes instructions for preparing and supplying these data to the program and a sample case in the appropriate format. The next section contains a discussion of the various types of output data obtained from the program and also of the output data from the sample case. A description of the error messages printed by the program is also included. Following that is a section containing miscellaneous information regarding the operation of the program with the CDC 6600 computing system.

The first appendix consists of a general discussion of the over-all logic structure of the program. The next appendix gives the Fortran nomenclature for the variables in the COMMON blocks of the program. The remaining appendices except the last provide detailed descriptions of the various components (main routine and subroutines) which make up the over-all program, one appendix for each component. The appendix for each new subroutine contains a presentation of the input and output variables, an internal Fortran nomenclature, a description of the step-by-step calculation procedure, and a Fortran listing of the subroutine. The last appendix contains a discussion of the method of calculation of the air distribution characteristics.

3.2 INPUT DATA

3.2.1 General Description

Program GASNOX requires the following input data in order to determine the nitric oxide emission level from an aircraft gas turbine engine.

a. Combustor Dimensions

1. V_P - Volume of the primary zone
2. X_L - Length of the intermediate zone (from the exit of the primary)

3. X_{END} - Distance from the primary zone exit to the exit from the combustor liner
4. R_X - Radius of liner at position X for canannular configuration
5. R_{X_I}, R_{X_O} - Inner and outer radii of liner at position X for annular configuration

b. Combustor Operating Conditions

1. T - Inlet temperature
2. P - Operating pressure
3. ϕ_P - Mass mean equivalence ratio in the primary zone (before fuel burns)
4. ϵ - Fraction of fuel entering the primary zone which burns in the zone
5. E_{rat} - Variable for altering $_P$ parametrically yet maintaining constant the over-all air-to-fuel ratio in the combustor
6. $(M_{a_X})_{\%}$ - Total mass per cent of air mixed with the product stream at position X in the liner
7. M_A - Total mass of air fed into the combustor liner
8. $\bar{\tau}_P$ - Mean primary zone residence time (applies only if V_P is set equal to zero)

c. Mixing Parameter for the Primary Zone

1. S_o - Degree of mixedness in the primary zone (where σ_o in the distribution function is given by $\sigma_o = S_o \bar{\Phi}_P$)

d. Kinetic Constants for each Mixture Ratio Element

1. R_1 - Forward reaction rate constant for the first reaction (see Section 2, Volume 2 or Ref 3)
2. R_6 - Forward reaction rate constant for the sixth reaction (see Section 2, Volume 2 or Ref 3)

3. K_1 - Ratio of forward reaction rate constants (see Section 2, Volume 2 or Ref 3)
4. K_2 - Ratio of forward reaction rate constants (see Section 2, Volume 2 or Ref 3)

e. Thermodynamic Properties for each Mixture Ratio Element
1. ρ - Density of the combustion products
2. T_f - Adiabatic flame temperature of the combustion products.

f. Equilibrium Compositions for each Mixture Ratio Element
1. $(NO)_e$ - Nitric oxide equilibrium mole fraction
2. $(CO)_e$ - Carbon monoxide equilibrium mole fraction
3. $(C_{(s)})_e$ - Solid carbon equilibrium mole fraction
4. $(CH_2)_e$ - Unburned hydrocarbons (exclusive of CO and $C_{(s)}$) equilibrium mole fraction.

The input data is read in three categories: 1) the kinetic, thermodynamic, and equilibrium data and the combustor inlet temperature and pressure; 2) the combustor airflow distribution and radius versus axial position; and 3) the remaining combustor dimensions, operating conditions, and the primary zone mixing parameter. With this structure there may be several sets of data in a given computer run. Figure 3 is a schematic representation of the data input structure.

3.2.2 Detailed Description of Input Data

The information required to prepare the input data for a case is furnished in the table given below. This information contains a description of each input item as well as a description of the form in which these items are written on input data sheets. The descriptions of the input items refer frequently to several points, relevant to the selection of input values, which are discussed in the following subsection. The discussions of these points provide additional detailed information useful in preparing the input data for any case.

The first input item read by Program GASNOX is the integer variable IDATA which identifies the number of sets of data in category 1. This input is then followed by the first set of category 1 data (see point a).

Line	Location	Input Item	Type of Number	Fortran Symbol	Description
1	1-6		Int	IDATA	Number of sets of data in category 1
2	1-72		A	SET(I)	Descriptive data identifying atomic composition of fuel and the turbine inlet temperature
3	1-14		A	SET(I)	Descriptive data of units of combustor inlet pressure
3	15-29	P	FP	PPP	Combustor inlet pressure (atm)
3	30-51		A	SET(I)	Descriptive data of set of kinetic constants used in calculation (see Volume 1, Table 2; descriptive data of k_s
3	52-66	k_s	FP	EKS	Fuel-to-air mass ratio at stoichiometric conditions
4	1-12	F_i	FP	FF(I)	Mixture ratio of an element
4	13-24	φ_i	FP	PHI(I)	Equivalence ratio of an element
4	25-36	ρ_i	FP	RHO(I)	Density of combustion products for an element (gm/cm^3)
4	37-48	T_i	FP	ATT(I)	Adiabatic flame temperature for an element (deg K)
4	49-60	$(NO_i)_e$	FP	BCON6(I)	Equilibrium mole fraction of NO for an element
4	61-72	$(CO_i)_e$	FP	BCON2(I)	Equilibrium mole fraction of CO for an element
5	1-12	$(C_{(s)i})_e$	FP	BCON1(I)	Equilibrium mole fraction of $C_{(s)}$ for an element
5	13-24	$(CH_{2_i})_e$	FP	CH2(I)	Equilibrium mole fraction of unburned hydrocarbons exclusive of $C_{(s)}$ and CO for an element
5	25-36	$(R_1)_i$	FP	R1(I)	Forward reaction rate for the first kinetic reaction (see Section 2, Volume 2 or Ref 3) ($gm\text{-}mole/cm^3\text{-}sec$) for an element

Line	Location	Input Item	Type of Number	Fortran Symbol	Description
5	37-48	$(R_6)_i$	FP	R6(I)	Forward reaction rate for the sixth kinetic reaction (see Section 2 , Volume 2 or Ref 3) (gm-mole/cm^3-sec) for an element
5	49-60	$(K_1)_i$	FP	EK1(I)	Ratio of forward reaction rate constants (see Section 2 , Volume 2 or Ref 3) for an element
5	61-72	$(K_2)_i$	FP	EK2(I)	Ratio of forward reaction rate constants (see Section 2, Volume 2 or Ref 3) for an element

Lines 4-5 are repeated for each of the 35 discrete mixture ratio elements specified in the distribution function. At the conclusion of this data, the integer variable KASE is read. KASE identifies the number of sets of data in category 2 that follow for the given set of data in category 1.

Line	Location	Input Item	Type of Number	Fortran Symbol	Description
74	1-6		Int	KASE	Number of sets of data in category 2
75	1-12	X	FP	AXX(J)	Axial position in the combustor (in)
75	13-24	$(M_{a_X})\%$	FP	APR(J)	Per cent of total mass of airflow in combustor liner at position X (cumulative)
75	25-36	R_X	FP	ARR(J)	Radius of liner at position X; applies only for canannular configuration (in) (see point b)
75	37-48	R_{X_I}	FP	ANR(J)	Inner radius of liner at position X; applies only for annular configuration (in) (see point b)
75	49-60	R_{X_0}	FP	ANNR(J)	Outer radius of liner at position X; applies only for annular configuration (in) (see point b)

Line 75 is repeated for each of 11 axial positions in the combustor. The first axial position must be taken as X = 0; that is, at the exit of the combustor primary zone.

There may be as many sets of data in category 3 for each set of data in category 2 as the user desires. The number of these data sets is read as the variable IN, on line 86.

Line	Location	Input Item	Type of Number	Fortran Symbol	Description
86	1-6		Int	IN	Number of sets of data in category 3

Following the data on line 86 is the data of category 3.

Line	Location	Input Item	Type of Number	Fortran Symbol	Description
87	1-12	V_P	FP	VP	Volume of primary zone (in^3) (see point c)
87	13-24	X_L	FP	XL	Length of intermediate zone (in)
87	25-36	X_{END}	FP	XEND	Length of intermediate zone and dilution zone (combined) (in)
87	37-48	ϕ_P	FP	EQUIV	Mass mean equivalence ratio in the primary zone (before fuel burns)
87	49-60	β	FP	BETA	Combustion efficiency in the primary zone
87	61-72	M_A	FP	TOTAIR	Total mass of air fed into the combustor liner (lb/sec)
88	1-12	S_o	FP	S	Degree of mixedness in the primary zone
88	13-24	E_{rat}	FP	ERAT	Variable for varying $\bar{\phi}_p$ parametrically yet maintaining constant air-to-fuel ratio in the combustor
88	25-36	$\bar{\tau}_p$	FP	TAUBAR	Mean primary zone residence time (applies only if V_p is set equal to zero) (see point c)

Lines 87-88 are repeated for each set of data in category 3 that the user wishes to specify.

3.2.3 Discussion of Input Data

Some important aspects to be considered in appropriately specifying the input data are discussed below. Reference to these discussions has been made in the preceding subsection in which the input format was described. The points referred to are as follows:

a. Data in category 1 (lines 2-73) are generated by Program NOXRAT described in Volume 2.

b. If a canannular configuration is tested, the variables R_{X_I} and R_{X_O} are set equal to zero. If an annular configuration is tested, the variable R_X is set equal to zero.

c. If the user chooses to specify the volume of the primary zone, V_p, then the mean primary zone residence time ($\bar{\tau}_p$) is set equal to zero in the input. $\bar{\tau}_p$ is then calculated by the program. If, on the other hand, the user chooses to specify $\bar{\tau}_p$, he must set V_p equal to zero in the input.

3.2.4 Description of Sample Case Input

Completed input data sheets are shown on pages 32 and 33. In this table lines 1-73 comprise the data and controls for category 1 (note: lines 6-73 are omitted for brevity); lines 74-85 comprise the data and controls for category 2; and lines 86-88 comprise the data and controls for category 3.

In this case, the fictitious combustor examined has an inlet temperature of 700 deg K and an operating pressure of 5.78 atm. The combustor is 10 inches in length from the exit of the primary zone, has a primary zone volume of 55 in^3, and is being operated with a mean primary zone equivalence ratio (before the fuel burns) of 0.9. The over-all air-to-fuel ratio is 92.

3.3 OUTPUT DATA

The output of Program GASNOX consists entirely of printed data. The printed data falls into two main categories: normal output, and

error messages with additional output. The normal output which is illustrated by the sample case included in the report, will be described first.

3.3.1 Normal Output

The information included in the normal output can be divided into the following categories:

1. General input data and miscellaneous calculated input data.
2. Elemental primary zone exit conditions from the converged solution.
3. Over-all primary zone exit conditions from the converged solution.
4. Over-all intermediate zone conditions at various axial positions in the zone from the converged solution.
5. Over-all dilution zone conditions at various axial positons in the zone from the converged solution.

A description of the items in each category is given below.

The normal output of a typical case begins with the items in category 1-- general input data and miscellaneous calculated input data. This data consists of:

a. Axial position in the combustor (where the origin is taken as the primary zone exit) (in).

b. Total mass per cent of air mixed with the product stream at position X.

c. Radius of liner at position X for canannular configuration or inner and outer radii of liner at position X for annular configuration (in).

d. The case number; this number corresponds to the set of combustor dimensions, operating conditions, and the primary zone mixing parameter for the given combustor airflow characteristics.

e. The cumulative normal distribution data.

f. The atomic formula of the fuel.

g. The combustor air inlet temperature (deg K).

h. The combustor operating pressure (atm).

i. A code number identifying the set of kinetic constants employed in the reaction scheme.

j. The value of the fuel-to-air mass ratio at stoichiometric conditions.

k. For each element in the distribution function: the mixture ratio (mass fuel to mass fuel and air); the equivalence ratio; the density of the combustion products in gm/cm^3; the adiabatic flame temperature of the combustion products in deg K; the equilibrium mole fraction of NO, CO, $C_{(s)}$, and CH_2 (unburned hydrocarbons); and the kinetic parameters R_1, R_6 (in gm-moles/cm^3-sec), K_1 and K_2 (dimensionless) defined in Section 2 of Volume 2.

l. The volume of the primary zone (in^3).

m. The length of the intermediate zone (in).

n. The length of the intermediate and dilution zone (combined) (in).

o. The mean primary zone equivalence ratio (before the fuel burns).

p. The combustion efficiency in the primary zone.

q. The total mass of air fed into the combustor liner (lb/sec).

r. The degree of mixedness in the primary zone.

s. The variable used for altering the mean primary zone equivalence ratio parametrically without changing the over-all air-to-fuel ratio in the combustor.

t. The total mass of fuel fed into the combustor (lb/hr).

u. The over-all air-to-fuel ratio in the combustor.

The normal output of a typical case continues with the items in category 2-- elemental primary zone conditions for the converged solution. These items, which begin after a statement describing them, consist of:

a. The mass fraction in the element.

b. The NO concentration in the element (ppm) (vol).

c. The cumulative sum of the NO formed up to and including the element (lb/sec).

d. The element number.

Only those elements with a finite rate of formation of NO are included in this output table.

The normal output of a typical case continues, after a statement describing the data, with the items in category 3-- over-all primary zone exit conditions from the converged solution. This data consists of:

a. The axial position in the combustor (in).

b. The mass mean primary zone equivalence ratio, accounting for the inefficiency of the primary zone combustion.

c. The mass mean exit temperature of the primary zone (deg F).

d. The mass mean density of the primary zone combustion products (lb/ft^3).

e. The mass mean primary zone residence time (msec).

f. The mass mean concentration of NO in the primary zone (ppm) (vol).

g. The mass mean concentration of NO in the primary zone, expressed as NO_2 (lb/1000 lb fuel burned).

h. The mass mean equilibrium concentration of $C_{(s)}$ in the primary zone (ppm) (vol).

i. The mass mean equilibrium concentration of $C_{(s)}$ in the primary zone (lb/1000 lb fuel burned).

j. The mass mean equilibrium concentration of CO in the primary zone (ppm) (vol).

k. The mass mean equilibrium concentration of CO in the primary zone (lb/1000 lb fuel burned).

l. The mass mean equilibrium concentration of unburned hydrocarbons (exclusive of CO and $C_{(s)}$) in the primary zone (ppm) (vol).

m. The mass mean equilibrium concentration of unburned hydrocarbons (exclusive of CO and $C_{(s)}$) in the primary zone (lb/1000 lb fuel burned).

n. The fuel loading ($lb/sec\text{-}ft^3\text{-}atm^2$).

The normal output of a typical case continues, after a statement describing the data, with the items in category 4-- over-all intermediate zone conditions at axial positions in the zone corresponding to the converged solution. This data consists of:

a. The axial position in the combustor (in).

b. The mass mean equivalence ratio, at the given axial station in the intermediate zone, accounting for the inefficiency of the primary zone combustion.

c. The mass mean exit temprature at the given axial station in the intermediate zone, (deg F).

d. The mass mean density of the combustion products at the given axial station in the intermediate zone (lb/ft^3).

e. The mass mean residence time of the combustion products from the combustor entrance to the given axial station in the intermediate zone (msec).

f. The mass mean concentration of NO at the given axial station in the intermediate zone (ppm) (vol).

g. The mass mean concentration of NO, expressed as NO_2, at the given axial station in the intermediate zone (lb/1000 lb fuel burned).

h. The mass mean equilibrium concentration of $C_{(s)}$ at the given axial station in the intermediate zone (ppm) (vol).

i. The mass mean equilibrium concentration of $C_{(s)}$ at the given axial station in the intermediate zone (lb/1000 lb fuel burned).

j. The mass mean equilibrium concentration of CO at the given axial station in the intermediate zone (ppm) (vol).

k. The mass mean equilibrium concentration of CO at the given axial station in the intermediate zone (lb/1000 lb fuel burned).

l. The mass mean equilibrium concentration of unburned hydrocarbons (exclusive of CO and $C_{(s)}$) at the given axial station in the intermediate zone (ppm) (vol).

m. The mass mean equilibrium concentration of unburned hydrocarbons (exclusive of CO and $C_{(s)}$) at the given axial station in the intermediate zone (lb/1000 lb fuel burned).

If the chemical rate of production of NO is frozen at any axial station in the intermediate zone, the program prints a message to that effect and proceeds with the dilution zone calculations and output.

The normal output of a typical case concludes, after a statement describing the data, with the items in category 5-- over-all dilution

zone conditions at axial positions in the zone corresponding to the converged solution. If the chemical rate of formation of NO was frozen at any axial station in the intermediate zone, only the dilution zone exit conditions are printed. The data in this category consists of:

a. The axial position in the combustor (in).
b. The mass mean equivalence ratio, at the given axial station in the dilution zone, accounting for the inefficiency of the primary zone combustion.
c. The mass mean exit temperature at the given axial station in the dilution zone (deg F).
d. The mass mean density of the combustion products at the given axial station in the dilution zone (lb/ft^3).
e. The mass mean residence time of the combustion products from the combustor entrance to the given axial station in the dilution zone (msec).
f. The mass mean concentration of NO at the given axial station in the dilution zone (ppm) (vol).
g. The mass mean concentration of NO, expressed as NO_2 at the given axial station in the dilution zone (lb/1000 lb fuel burned).
h. The mass mean equilibrium concentration of $C_{(s)}$ at the given axial station in the dilution zone (ppm) (vol).
i. The mass mean equilibrium concentration of $C_{(s)}$ at the given axial station in the dilution zone (lb/1000 lb fuel burned).
j. The mass mean equilibrium concentration of $C_{(s)}$ at the given axial station in the dilution zone (ppm) (vol).
k. The mass mean equilibrium concentration of CO at the given axial station in the dilution zone (lb/1000 lb fuel burned).
l. The mass mean equilibrium concentration of unburned hydrocarbons (exclusive of CO and $C_{(s)}$) at the given axial station in the dilution zone (ppm) (vol).
m. The mass mean equilibrium concentration of unburned hydrocarbons (exclusive of CO and $C_{(s)}$) at the given axial station in the dilution zone (lb/1000 lb fuel burned).

If the chemical rate of prediction of NO is frozen at any axial station in the dilution zone, the program prints a message to that

effect after completing the dilution zone calculations and printing the output at the axial position that corresponds to the combustor exit.

3.3.2 Error Messages and Additional Output

In addition to the normal output, various messages may appear in the output of a case. These messages either indicate that difficulty has been encountered during execution of the case or that the user has specified the printing of intermediate output to examine progress in the iterations. The messages are considered below in the order of their appearance in the program.

a. If intermediate output is requested by the user, the program will print the value of the total mass contained in each mixture ratio element and the value of the parameters that define the range of the mass distribution function. These values are printed in Subroutine ZMASS; they are printed for each converged axial position in the combustor.

b. If, in calculating the values of $(\alpha_{\sigma_T})_i$, the number of iterations on a given element equal ten, the program prints the number of iterations and the last value of $(\alpha_{\sigma_T})_i$. This is a nonfatal error as the program assumes the value of $(\alpha_{\sigma_T})_i$ to be the last value calculated. The error message is printed in Subroutine PRCALC. This error is caused by limiting the number of iterations to ten; it can be relieved by increasing the limit.

c. POTENTIAL ERROR DUE TO LACK OF CONVERGENCE, SUMTNO(I) = ±X.XXXXXXXXE±XX PRIOR VALUE OF SUMTNO(I) = ±X.XXXXXXXXE±XX I = XXX

   This message is printed in Subroutine PRCALC for a primary zone element that fails to satisfy convergence criteria after five iterations. This is a nonfatal error as the program assumes that the value of SUMTNO(I) is the last value calculated. The error is caused by limiting the number of iterations to five; it can be remedied by increasing the limit.

d. If intermediate output is requested by the user, the program will print the value of the nitric oxide content of each mixture ratio element for each converged axial position in the combustor. These values are printed in Subroutine PRINTS.

e. If the number of iterations attempting to satisfy the mixing criteria equal 40 for any mixture ratio element at any axial station in the intermediate zone, Subroutine ZINTER will print the most recent value of E_i, and the number of iterations. This is a fatal condition to the program causing immediate termination of the calculations. This procedure is a safety control to keep the program from continuing into an indefinite loop; it is likely caused by some trouble in the calculation of element masses and can only be remedied by detailed examination of the flow rates into and out of each mass element.

f. X(CM) = +X.XXXXXXE±XX J = XX
AVE. RHO(GM/CC) = +X.XXXXXE±XX
AVE. NO(GM/GM) = +X.XXXXXE±XX
This message is printed from Subroutine ZINTER at the end of each iteration loop in the intermediate zone if intermediate output is requested by the user. The meaning of the message is quite clear; both the density and nitric oxide concentrations are mass averages. J is the number of iterations.

g. RUNGE-KUTTA ITERATION FAILED TO CONVERGE TO SPECIFIED LIMIT,
DIFNO = ±X.XXXXXE±XX N = XXXX X = CMS
This nonfatal message is printed by Subroutine ZINTER at each axial position in the intermediate zone where convergence criteria on the NO iterations are not satisfied. N here is the number of steps each major step is divided into for the last iteration; DIFNO identifies the difference in the calculated nitric oxide levels at the end of the major step down the combustor to position X. There are two possible reasons for the appearance of the message:

1. The number of steps allowed in the Runge-Kutta integration are inadequate.

2. The convergence limit is too narrow.

Relaxation of either of these control criteria will eliminate the iteration difficulty.

h. X(CM) = +X.XXXXXE+XX J = XX AVE.RHO
GM/CC) = +X.XXXXXE+XX AVE.NO = +X.XXXXXE+XX
+X.XXXXXE+XX +X.XXXXXE+XX

This message is printed from Subroutine DILUTE at the end of each iteration in the dilution zone if intermediate output is requested by the user. The meaning of the message is quite clear except for the last two variables printed; these variables are rate of change of nitric oxide mass fraction with position due to chemical reaction and, dilution, respectively. Both the density and nitric oxide concentrations are mass averages. J is the number of iterations.

i. If intermediate output is requested by the user, Subroutine DILUTE prints the difference between the calculated nitric oxide levels for the last two iterations at the end of each major step down the combustor. In addition, DILUTE also prints the number of integration steps each major step is divided into for the last iteration.

j. RUNGE-KUTTA ITERATION FAILED TO CONVERGE TO SPECIFIED LIMIT.
DIFNO = +X.XXXXXE+XX N = XXXX X = +X.XXXXXE+XX

This nonfatal message is printed by Subroutine DILUTE at each axial position in the dilution zone where convergence criteria on the NO iterations are not satisfied. N here is the number of steps each major step is divided into for the last iteration; DIFNO identifies the difference in the calculated nitric oxide levels at the end of the major step down the combustor to position X. There are two possible reasons for the appearance of the message:

1. The number of steps allowed in the Runge-Kutta integration are inadequate.
2. The convergence limit is too narrow.

Relaxation of either of these control criteria will eliminate the iteration difficulty.

3.3.3 Description of Sample Case Output

The output from the fictitious sample case described on pages 33 and 34 is presented on pages 35-42. The data on pages 35-38 represents the input data for this fictitious case while calculated results are shown on pages 39-42. From the data it is seen that the mean primary zone residence time for the combustor is 2 msec; and, in that time, a mass average concentration of 300 ppm (vol) of nitric oxide has been formed. Within a distance of 1.5 inches down the combustor intermediate zone, the chemical rate of formation of nitric oxide is negligible in comparison with the amount of nitric oxide previously formed. Consequently, only the dilution of the total nitric oxide formed to that point is important to the final emission figure of 73 ppm (vol).

3.4 MISCELLANEOUS OPERATIONAL INFORMATION

Program GASNOX occupies approximately 20,000 core locations during loading and approximately 12,000 core locations during execution on the CDC 6600 computer. Actual program length is approximately 7100 core locations. Hence, the total storage requirement for this program is comfortably within the CDC 6600 core capacity of 131,000 locations.

The execution time for Program GASNOX depends upon the characteristics of the particular combustor being analyzed. It has been found, however, that a typical case will require approximately 10 to 15 seconds of central processor time on the CDC 6600 with another 1 to 2 systems seconds necessary to satisfy input/output requirements. Approximately 12 systems seconds are required to load and compile the program.

There are no known sources of convergence difficulties in the program save the limits imposed on the number and accuracy of the Runge-Kutta integrations. These requirements are adequate for most applications of the program; they are neither too restrictive to cause convergence difficulties nor too loose to permit an abundance of interations and excessive computer costs.

NORTHERN RESEARCH AND ENGINEERING CORPORATION

3.5 DATA INPUT SHEET

ENGINEER: RDS **PROJECT:** NOx from Gas Turbine Combustors **PROJECT NO:** 1162

TITLE: Sample to Illustrate the Use of Program GASNOX **SHEET:** 1 **OF** 2

LOCATION

	1–12	13–24	25–36	37–48	49–60	61–72
Line 1	1					
Line 2	FUEL=, C 1.0	0000000E+00 H	1.94230000E	+00 INLET AI	R T.(K.)= 7.	00000000E+02
Line 3	PRESS.. (ATM)	= 5.7800000	0E+001,CODE=	2, PHI STOICH	.= 6.795228	49E-02
Line 4	8.48679E-04	1.24999E-02	2.78586E-03	7.32406E+02	6.54668E-07	0.
Line 5	0.	3.36139E-06	0.	0.	1.00000E+35	1.00000E+35
.						
.						
.						
Line 74	1					
Line 75	0.0	20.0	3.0	0.0	0.0	
Line 76	1.0	30.0	3.0	0.0	0.0	
Line 77	2.0	35.0	3.0	0.0	0.0	
Line 78	3.0	40.0	3.0	0.0	0.0	
Line 79	4.0	45.0	3.0	0.0	0.0	
Line 80	5.0	50.0	3.0	0.0	0.0	
Line 81	6.0	60.0	3.0	0.0	0.0	
Line 82	7.0	70.0	3.0	0.0	0.0	
Line 83	8.0	80.0	3.0	0.0	0.0	
Line 84	9.0	90.0	3.0	0.0	0.0	
Line 85	10.0	100.0	3.0	0.0	0.0	
Line 86	1					

NORTHERN RESEARCH AND ENGINEERING CORPORATION

3.5 DATA INPUT SHEET

ENGINEER: RDS PROJECT: NOx from Gas Turbine Combustors PROJECT NO: 1162

TITLE: Sample to Illustrate the Use of Program GASNOX SHEET: 2 OF 2

LOCATION

	1 6	7 12	13 18	19 24	25 30	31 36	37 42	43 48	49 54	55 60	61 66	67 72
Line 87		55.0		7.0		10.0		0.8		0.9		5.0
Line 88		0.5		1.0		0.0						

3.6 SAMPLE CASE OUTPUT

COMBUSTOR AIR FLOW CHARACTERISTICS

DISTANCE INCHES	PERCENTAGE AIR FLOW	CAN RADIUS INCHES	ANNULAR INNER RADIUS INCHES	ANNULAR OUTER RADIUS INCHES
0.	2.00000E+01	3.00000E+00	-0.	-0.
1.00000E+00	3.00000E+01	3.00000E+00	-0.	-0.
2.00000E+00	3.50000E+01	3.00000E+00	-0.	-0.
3.00000E+00	4.00000E+01	3.00000E+00	-0.	-0.
4.00000E+00	4.50000E+01	3.00000E+00	-0.	-0.
5.00000E+00	5.00000E+01	3.00000E+00	-0.	-0.
6.00000E+00	6.00000E+01	3.00000E+00	-0.	-0.
7.00000E+00	7.00000E+01	3.00000E+00	-0.	-0.
8.00000E+00	8.00000E+01	3.00000E+00	-0.	-0.
9.00000E+00	9.00000E+01	3.00000E+00	-0.	-0.
1.00000E+01	1.00000E+02	3.00000E+00	-0.	-0.

CASE NO. = 1

CUMULATIVE NORMAL DISTRIBUTION DATA

ZP	CUMDIS	ZP	CUMDIS	ZP	CUMDIS	ZP	CUMDIS	ZP	CUMDIS	ZP	CUMDIS	ZP	CUMDIS
0.00	.5000	.50	.6915	1.00	.8413	1.50	.9332	2.00	.9772	2.50	.9938	3.00	.9987
.05	.5199	.55	.7088	1.05	.8531	1.55	.9394	2.05	.9798	2.55	.9946	3.05	.9989
.10	.5398	.60	.7257	1.10	.8643	1.60	.9452	2.10	.9821	2.60	.9953	3.10	.9990
.15	.5596	.65	.7422	1.15	.8749	1.65	.9505	2.15	.9842	2.65	.9960	3.15	.9992
.20	.5793	.70	.7580	1.20	.8849	1.70	.9554	2.20	.9861	2.70	.9965	3.20	.9993
.25	.5987	.75	.7734	1.25	.8944	1.75	.9599	2.25	.9878	2.75	.9970	3.25	.9994
.30	.6179	.80	.7881	1.30	.9032	1.80	.9641	2.30	.9893	2.80	.9974	3.30	.9995
.35	.6368	.85	.8023	1.35	.9115	1.85	.9678	2.35	.9906	2.85	.9978	3.35	.9996
.40	.6554	.90	.8159	1.40	.9192	1.90	.9713	2.40	.9918	2.90	.9981	3.40	.9997
.45	.6736	.95	.8289	1.45	.9265	1.95	.9744	2.45	.9929	2.95	.9984	3.45	.9997

EQUILIBRIUM DATA

FUEL= C 1.00000000E+00H 1.94230000E+00 INLET AIR T.(K)= 7.00000000E+02 PRESS.(ATM)= 5.78000000E+00
IOCODE= 2PHI STOICH.= 6.79522849E-02

THE FOLLOWING DATA TABLE CONTAINS THE THERMODYNAMIC PROPERTIES,KINETIC RATE CONSTANTS,AND EQUILIBRIUM COMPOSITIONS FOR EACH PRESCRIBED EQUIVALENCE RATIO. FOR EACH ELEMENT THESE PROPERTIES ARE,IN ORDER OF PRINTING...MIXTURE RATIO,EQUIVALENCE RATIO, DENSITY,ADIABATIC FLAME TEMPERATURE,NO,CO,C(S),AND CH2(UNBURNED HYDROCARBONS) EQUILIBRIUM MOLE FRACTION,AND THE KINETIC PARAMETERS P1,P6,K1,AND K2.

ELEMENT						
1	8.48679E-04	1.24999E-02	2.79586E-03	7.32406E+02	6.54668E-07	0.
	0.	3.34130E-06	0.	0.	1.00000E+35	1.00000E+35
2	6.74914E-03	9.99966E-02	2.17492E-03	9.55679E+02	1.99330E-05	0.
	0.	2.47305E-05	0.	0.	1.00000E+35	1.00000E+35
3	1.47062E-02	2.50028E-01	1.56378E-03	1.30444E+03	3.78239E-04	0.
	0.	6.61614E-05	0.	1.07179E-14	1.00000E+35	1.19999E+00
4	2.44600E-02	3.99987E-01	1.25992E-03	1.61914E+03	1.68857E-03	1.65033E-06
	0.	1.34784E-04	0.	2.66082E-11	1.00000E+35	8.75547E-01
5	3.28633E-02	5.00057E-01	1.12540E-03	1.91245E+03	3.12182E-03	2.06868E-05
	0.	1.30121E-04	0.	5.76354E-10	1.00000E+35	7.22611E-01
6	3.40230E-02	5.49945E-01	1.07110E-03	2.00413E+03	3.92834E-03	5.84645E-05
	0.	1.42619E-04	0.	1.01368E-09	1.00000E+35	6.45426E-01
7	3.91720E-02	5.99980E-01	1.02322E-03	2.09287E+03	4.74022E-03	1.48130E-04
	0.	1.55059E-04	0.	5.33511E-09	1.00000E+35	5.69216E-01
8	4.23015E-02	6.50015E-01	9.80949E-04	2.17817E+03	5.49984E-03	3.41685E-04
	0.	1.67397E-04	0.	1.27003E-08	1.00000E+35	4.95151E-01
9	4.54099E-02	7.00050E-01	9.43571E-04	2.15985E+03	6.14446E-03	7.27500E-04
	0.	1.79619E-04	0.	2.41425E-08	1.00000E+35	4.23914E-01
10	4.04890E-02	7.49938E-01	9.10677E-04	2.33607E+03	6.60557E-03	1.44131E-03
	0.	1.91671E-04	0.	4.47134E-08	1.00000E+35	3.56233E-01
11	5.15573E-02	7.99973E-01	8.81754E-04	2.30709E+03	6.81936E-03	2.68638E-03
	0.	2.03594E-04	2.74234E-06	7.36144E-08	7.26704E-01	2.92195E-01
12	5.46060E-02	8.50008E-01	8.56737E-04	2.37094E+03	6.72783E-03	4.72358E-03
	0.	2.15325E-04	5.02999E-06	9.72566E-09	7.20039E-01	2.32543E-01
13	5.76350E-02	9.00043E-01	8.35575E-04	2.42585E+03	6.29833E-03	7.86600E-03
	0.	2.26846E-04	7.80726E-06	1.10592E-07	6.93156E-01	1.77941E-01
14	6.06350E-02	9.49931E-01	8.18377E-04	2.46962E+03	5.54070E-03	1.24355E-02
	0.	2.37952E-04	1.00976E-05	1.44188E-07	6.48543E-01	1.29399E-01
15	6.36264E-02	9.99966E-01	8.05235E-04	2.50010E+03	4.51510E-03	1.87793E-02
	0.	2.48760E-04	1.04590E-05	7.02971E-08	5.88988E-01	8.78079E-02
16	6.45982E-02	1.05000E+00	7.94486E-04	2.51471E+03	3.36176E-03	2.70973E-02
	0.	2.59161E-04	8.94346E-06	4.48228E-08	5.18732E-01	5.47617E-02
17	6.95511E-02	1.10004E+00	7.92234E-04	2.51221E+03	2.27836E-03	3.72910E-02
	0.	2.69083E-04	5.93944E-06	2.12770E-08	4.44162E-01	3.12993E-02
18	7.24747E-02	1.14992E+00	7.91985E-04	2.49484E+03	1.43390E-03	4.87489E-02
	0.	2.78514E-04	3.19693E-06	7.00724E-09	3.73572E-01	1.68128E-02
19	7.53925E-02	1.19996E+00	7.94438E-04	2.46617E+03	8.64265E-04	6.07089E-02
	0.	2.87580E-04	1.49561E-06	2.59183E-09	3.12464E-01	9.78572E-03
20	7.82900E-02	1.24999E+00	7.99116E-04	2.43173E+03	5.13435E-04	7.24768E-02
	0.	2.96344E-04	6.51134E-07	7.55146E-10	2.62566E-01	4.60619E-03
21	8.11695E-02	1.30003E+00	8.04691E-04	2.39427E+03	3.05031E-04	8.36946E-02
	0.	3.04417E-04	2.73122E-07	2.33653E-10	2.22590E-01	2.45509E-03

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22	8.80224E-02	1.34992E+00	8.10931E-04	2.35558E+03	1.82499E-04	9.41889E-02
	0.	3.13014E-04	1.12745E-07	6.43862E-11	1.90627E-01	1.33707E-03
23	8.86644E-02	1.39995E+00	8.17655E-04	2.31634E+03	1.09762E-04	1.03992E-01
	0.	3.21003E-04	4.59405E-08	1.07240E-11	1.64487E-01	7.40730E-04
24	8.96924E-02	1.44999E+00	8.24725E-04	2.27711E+03	6.64275E-05	1.13098E-01
	0.	3.28774E-04	1.85838E-08	0.	1.43457E-01	1.00000E+35
25	9.24766E-02	1.45958E+00	8.32014E-04	2.23850E+03	4.05806E-05	1.21485E-01
	0.	3.36271E-04	0.	0.	1.00000E+35	1.00000E+35
26	9.50429E-02	1.59965E+00	8.47461E-04	2.16181E+03	1.51517E-05	1.36718E-01
	0.	3.50819E-04	0.	0.	1.00000E+35	1.00000E+35
27	1.06265E-01	1.74976E+00	8.72379E-04	2.08044E+03	3.46315E-06	1.56206E-01
	0.	3.71338E-04	0.	0.	1.00000E+35	1.00000E+35
28	1.14330E-01	1.89986E+00	8.99480E-04	1.94343E+03	7.69367E-07	1.72789E-01
	0.	3.90533E-04	0.	0.	1.00000E+35	1.00000E+35
29	1.22269E-01	2.04997E+00	9.29028E-04	1.84049E+03	1.61174E-07	1.87362E-01
	0.	4.08708E-04	0.	0.	1.00000E+35	1.00000E+35
30	1.30057E-01	2.20007E+00	9.61306E-04	1.74126E+03	3.09300E-08	2.00521E-01
	0.	4.26220E-04	0.	0.	1.00000E+35	1.00000E+35
31	1.37708E-01	2.35018E+00	9.96699E-04	1.64540E+03	0.	2.12683E-01
	0.	4.43885E-04	0.	0.	1.00000E+35	1.00000E+35
32	1.45224E-01	2.50028E+00	1.03567E-03	1.55259E+03	0.	2.24167E-01
	0.	4.64745E-04	0.	0.	1.00000E+35	1.00000E+35
33	1.52614E-01	2.65039E+00	1.07876E-03	1.46259E+03	0.	2.35235E-01
	0.	5.06610E-04	0.	0.	1.00000E+35	1.00000E+35
34	1.59876E-01	2.80049E+00	1.12620E-03	1.37607E+03	0.	2.46025E-01
	0.	7.27035E-04	0.	0.	1.00000E+35	1.00000E+35
35	1.67014E-01	2.95060E+00	1.17095E-03	1.30429E+03	0.	2.55129E-01
	0.	3.09731E-03	0.	0.	1.00000E+35	1.00000E+35

```
                         THE REST OF THE INPUT VARIABLES

THE VOLUME OF THE PRIMARY ZONE IS  5.50000E+01 CU.IN.

THE LENGTH OF THE INTERMEDIATE ZONE IS  7.00000E+00 IN.

THE LENGTH OF THE INTERMEDIATE ZONE AND DILUTION ZONE(COMBINED) IS  1.00000E+01 IN.

THE MEAN PRIMARY ZONE EQUIVALENCE RATIO IS  8.00000E-01

THE COMBUSTION EFFICIENCY IN THE PRIMARY ZONE IS  9.00000E-01

THE TOTAL MASS OF AIR FED INTO THE COMBUSTOR IS  5.00000E+00 LB./SEC.

THE DEGREE OF MIXEDNESS IS  6.00000E-01

ERAT =  1.00000E+00

THE MEAN PRIMARY ZONE RESIDENCE TIME(ONLY APPLIES IF THE VOLUME OF THE PRIMARY ZONE IS ZERO IN INPUT) IS  0.        SEC.

THE COMPUTED TOTAL MASS OF FUEL FED INTO THE COMBUSTOR IS  1.95703E+02 LB./HR.

THE COMPUTED OVERALL AIR-TO-FUEL RATIO IS  9.19763E+01
```

PRIMARY ZONE EXIT CONDITIONS

MASS FRACTION	NO PPM(VOL)	TOTAL NO LB/SEC	ELEMENT NO.
1.09486E-02	0.	0.	1
3.56556E-02	0.	0.	2
7.77667E-02	7.04282E-07	5.60269E-14	3
9.63209E-02	1.38132E-03	1.36357E-10	4
7.03778E-02	3.65236E-02	2.74591E-09	5
5.09434E-02	1.33395E-01	9.71739E-09	6
5.33612E-02	4.09180E-01	3.10903E-08	7
5.49167E-02	1.06376E+00	9.17573E-08	8
5.52783E-02	2.39028E+00	2.24921E-07	9
5.49666E-02	4.64425E+00	4.81696E-07	10
5.35626E-02	3.79710E+02	2.12928E-05	11
5.13500E-02	6.81170E+02	5.76047E-05	12
4.93185E-02	1.03452E+03	1.00530E-04	13
4.48685E-02	1.24321E+03	1.67436E-04	14
4.09380E-02	1.30218E+03	2.27969E-04	15
3.67762E-02	1.07783E+03	2.62517E-04	16
3.25742E-02	7.27704E+02	2.84766E-04	17
2.83198E-02	4.12037E+02	2.99702E-04	18
2.44663E-02	2.04478E+02	3.01825E-04	19
2.05762E-02	9.32373E+01	3.03797E-04	20
1.72139E-02	4.02463E+01	3.04496E-04	21
1.41327E-02	1.68516E+01	3.04740E-04	22
1.15454E-02	6.81227E+00	3.04820E-04	23
9.22063E-03	2.74941E+00	3.04846E-04	24
5.22083E-03	0.	3.04846E-04	25

THIS IS THE MAIN PRINTOUT FOR THE PRIMARY ZONE

X(IN.)	PHI AVE.	T DEG F	RHO AVE. (LB/CUFT)	TAU AVE. MSEC	NO PPM (VOL)	NO2 LBS PER 1000 LB FUEL BURNED	C(S) PPM (VOL)	C(S) LBS PER 1000 LB FUEL BURNED	CO PPM (VOL)	CO LBS PER 1000 LB FUEL BURNED	CH2 PPM (VOL)	CH2 LBS PER 1000 LB FUEL BURNED
0.00	.72	3235	.0658	2.00	3.000E+02	9.617E+00	0.	0.	1.453E+04	2.836E+02	1.820E+02	1.776E+00

THE FUEL LOADING IS 5.11234E-02 LB./SEC.-CU.FT.-ATMO.-ATMO.

THIS IS THE MAIN PRINTOUT FOR THE INTERMEDIATE ZONE

X(IN.)	PHI AVE.	T DEG F	CHC AVE. LB/CUFT	TAU AVE. MSEC	NO PPM (VOL)	NO2 LBS PER 1000 LB FUEL BURNED	C(S) PPM (VOL)	C(S) LBS PER 1000 LB FUEL BURNED	CO PPM (VOL)	CO LBS PER 1000 LB FUEL BURNED	CH2 PPM (VOL)	CH2 LBS PER 1000 LB FUEL BURNED
.30	.64	3124	.0677	2.27	2.886E+02	1.036E+01	0.	0.	6.433E+03	1.406E+02	1.642E+02	1.795E+00
.60	.57	2962	.0712	2.53	2.717E+02	1.085E+01	0.	0.	2.845E+03	6.616E+01	1.479E+02	1.797E+00
.90	.52	2806	.0746	2.78	2.502E+02	1.103E+01	0.	0.	1.221E+03	3.275E+01	1.343E+02	1.801E+00
1.20	.49	2716	.0764	3.01	2.370E+02	1.112E+01	0.	0.	6.672E+02	1.905E+01	1.268E+02	1.809E+00
1.50	.47	2656	.0775	3.24	2.264E+02	1.111E+01	0.	0.	4.071E+02	1.216E+01	1.218E+02	1.819E+00

---------NITRIC OXIDE REACTION FROZEN AT THIS POINT-----------------

THIS IS THE MAIN PRINTOUT FOR THE DILUTION ZONE

X(IN.)	PHI AVE.	T DEG F	RHO AVE. LB/CUFT	TAU AVE. MSEC	NO PPM (VOL)	NO2 LBS PER 1000 LB FUEL BURNED	C(S) PPM (VOL)	C(S) LBS PER 1000 LB FUEL BURNED	CO PPM (VOL)	CO LBS PER 1000 LB FUEL BURNED	CH2 PPM (VOL)	CH2 LBS PER 1000 LB FUEL BURNED
10.00	.16	1513	.0976	7.27	7.288E+01	1.051E+01	0.	0.	0.	0.	4.260E+01	1.870E+00

4. REFERENCES

1. Danckwerts, P. V., "Continuous Flow Systems, Distribution of Residence Times", Chemical Engineering Science, vol. 1, 1953, pp. 1-13.

2. Jackson, S. R. and Odgers, J., "Factors Influencing Heat Release in Combustion Chambers and Consideration of the Related Materials and Structures", Combustion in Advanced Gas Turbine Systems, Proceedings of an International Propulsion Symposium held at the College of Aeronautics, Cranfield, England, April, 1967.

3. Fletcher, R. S. and Heywood, J. B., A Model for Nitric Oxide Emissions from Aircraft Gas Turbine Engines (AIAA Paper No. 71-123), American Institute of Aeronautics and Astronautics, Presented at the AIAA 9th Aerospace Sciences Meeting, New York, N.Y., January 25-27, 1971.

5. FIGURES

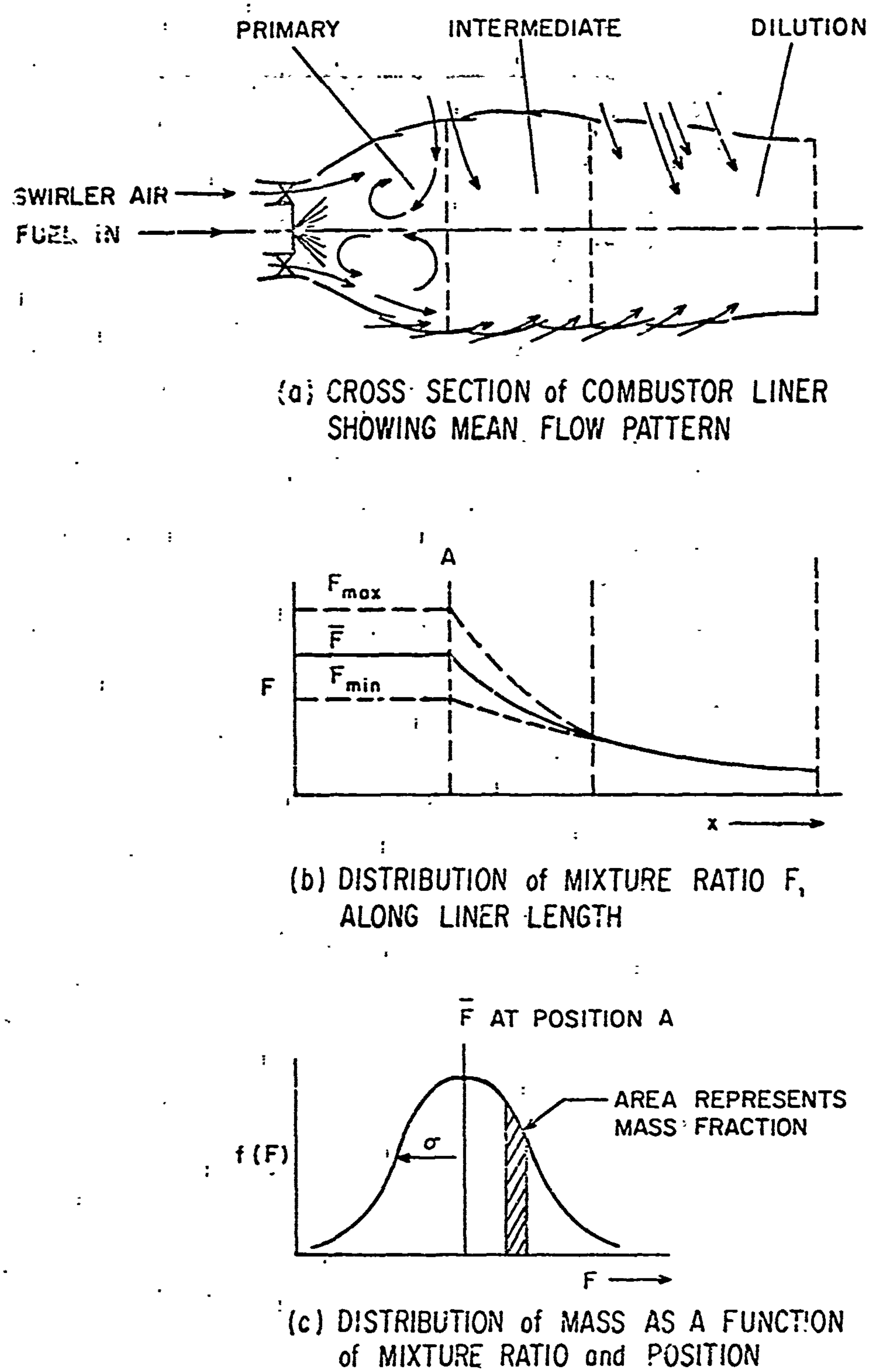
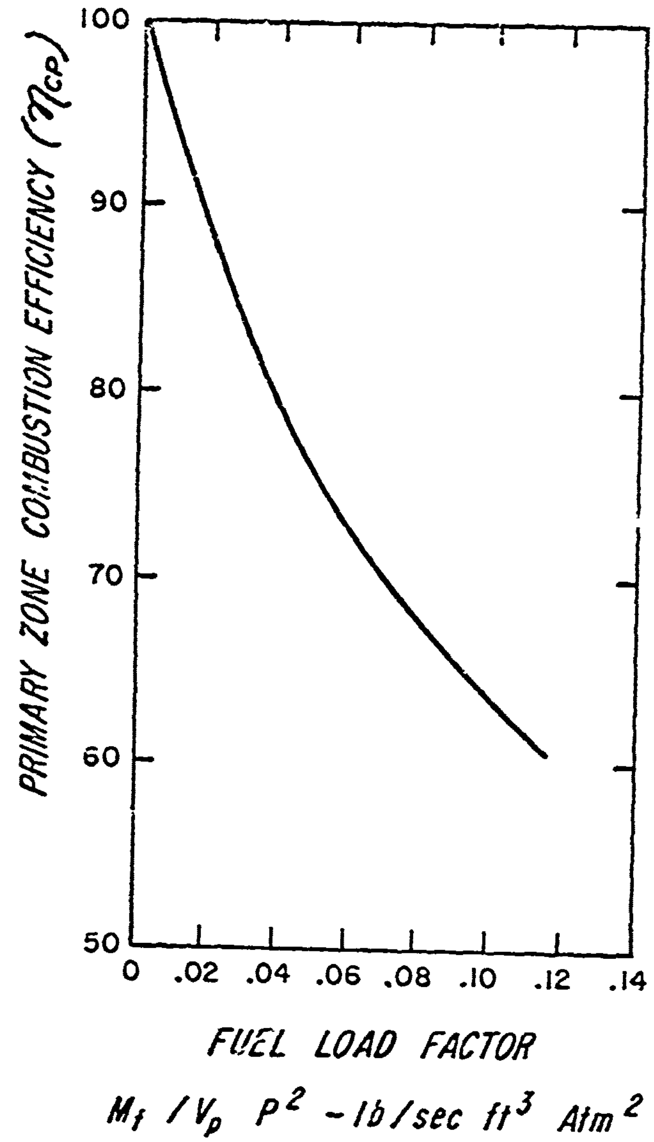


Figure 1 ASSUMED FLOW AND DISTRIBUTION PATTERNS THROUGHOUT COMBUSTOR LINER



REPRODUCED FROM REFERENCE 2

Figure 2 PRIMARY ZONE COMBUSTION EFFICIENCY CORRELATION

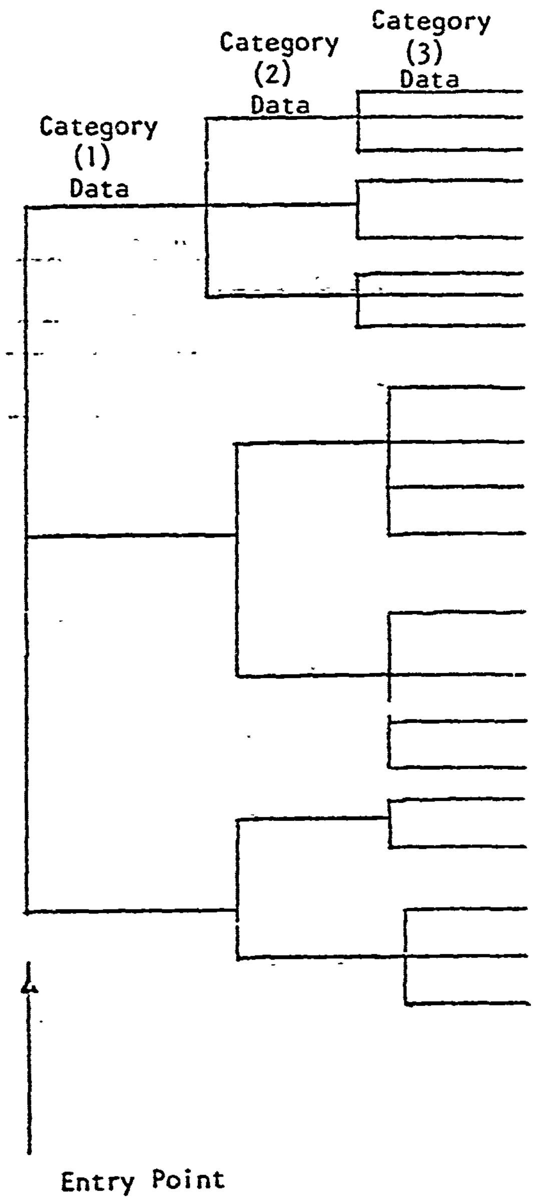


FIGURE 3 - SCHEMATIC REPRESENTATION OF INPUT STRUCTURE

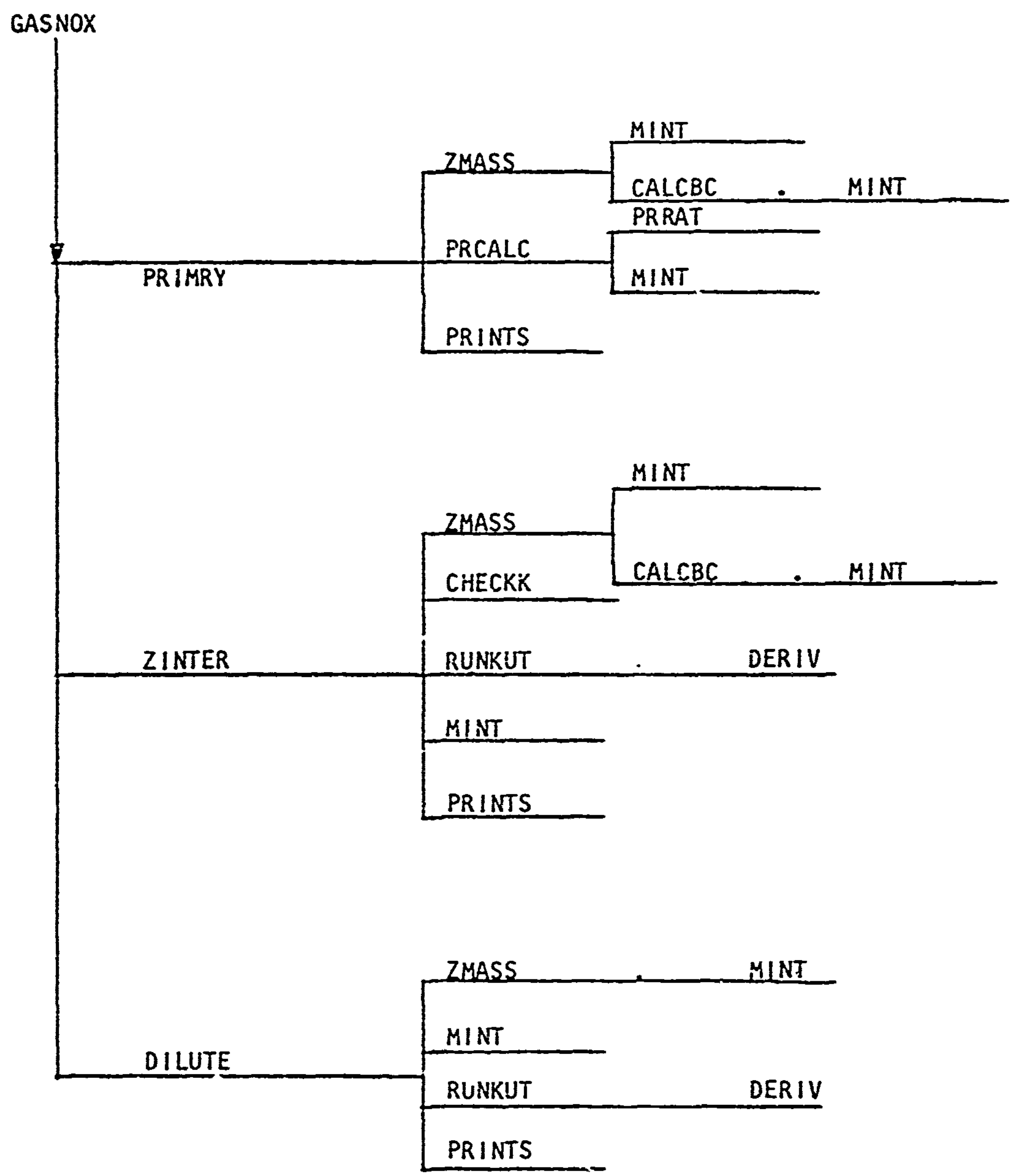


FIGURE 4 - MODULAR TREE DIAGRAM

6. NOMENCLATURE

Symbols	Description
A'	Preexponential factor in Arthenus equation
A	Total cross-sectional area of combustor liner
A_1	Model constant in equation A-15
A_2	Model constant in equation A-24
A_3	Model constant in equation A-24
b	Coefficient in combustor efficiency parameter
C	Normalizing factor in distribution function
E	Activation energy
f	Fraction of mass δm
F	Mixture ratio, (fuel mass/total mass)
k	Reaction rate constant
K	Fraction of mass δm leaving control value over δx
L	Length of intermediate zone
$\dot{m}$	Total mass flow rate in combustor liner
$\ddot{m}_a$	Mass flow rate of diluent air per unit length
M_{NO}	Moleculer weight of nitric oxide
$[NO]$	Mass fraction of nitric oxide, (Mass NO/total mass)
$[\Delta NO]$	$\{[NO]' - [NO]_x\}$
P	Pressure
$\dot{r}$	Rate of formation of nitric oxide per unit volume
R	Gas constant
R_n	Equilibrium rate of reaction
$\dot{R}$	$d/dx\,(\epsilon\,\delta m)$
t	Time
T	Temperature
V	Velocity
$\bar{V}$	Characteristic combustor velocity
V_p	Volume of primary zone
x	Axial distance
δA	Cross-sectional area of element with mixture ratio F
δm	Mass rate of element with mixture ratio F
δF	Range of F about F in element with mass
α	Nitric oxide concentration as fraction of equilibrium

Symbols	Description
ε	Fractional mass flow of unburned fuel, $m_{fu/m}$
β	Fraction of fuel burned in primary zone
σ	Standard deviation
ρ	Density
τ	Residence time
θ	Combustion efficiency parameter

Subscripts	Description
a	Dilution air
f	Total fuel
fu	Unburned fuel
F	With characteristic mixture ratio F
i	i^{th} element in series
L	State below that indicated by *
p	Condition in primary zone
t	With characteristic residence time t
u	State above that indicated by *
o	Condition at entrance to intermediate zone

Superscripts	Description
$(\ )'$	Condition at entry to control volume
$(\ )''$	Condition at exit from control volume
$(\ )^*$	Condition of combustor products entrained into control volume
$(\bar{\ })$	Mass average value

7. APPENDICES

APPENDIX I - OVER-ALL PROGRAM LOGIC

Program GASNOX consists of a main routine and twelve subroutines. The subroutines are PRIMRY, ZINTER, DILUTE, PRCALC, PRRAT, CHECKK, CALCBC, RUNKUT, DERIV, MINT, ZMASS, and PRINTS. Information is transmitted within the computer program through blocks of COMMON and as arguments of certain subroutines. The over-all control of the programmed calculation procedure is maintained by the main routine.

The logic flow begins at the start of the main routine where the input data is read and then printed. Subroutine PRIMRY, which controls the combustor primary zone calculations, is then called.

The primary zone is modeled as a partially stirred reactor, with the variations in gas composition, temperature, and residence time taken into account statistically. Thus, PRIMRY first calls Subroutine ZMASS to calculate element masses. ZMASS, in turn, calls Subroutines MINT and CALCBC. MINT provides interpolated values of tabulated functions of one variable assuming a linear relationship between the adjacent tabular entries. CALCBC calculates values of the mass flow coefficient at each axial station of the combustor primary and intermediate zones. CALCBC also calls Subroutine MINT. After calling ZMASS, Subroutine PRIMRY calls Subroutines PRCALC and PRINTS. PRCALC controls and calculates the average nitric oxide level in the primary zone for each specified mixture ratio element in the mass distribution function. PRCALC calls Subroutines PRRAT and MINT to conduct its calculations; PRRAT solves the analytical expression relating the elemental nitric oxide concentration to the elapsed time in the primary zone. PRINTS provides the written output of the calculated results of the program.

Having completed the primary zone calculations, GASNOX calls Subroutine ZINTER to perform and control the intermediate zone analysis <u>if</u> the primary zone mixing parameter is other than zero. If the mixing parameter is set at zero, GASNOX skips over the intermediate zone calculations and proceeds with dilution zone calculations via Subroutine DILUTE.

The intermediate zone of the combustor is divided into a series of finite length axial elements in which the heterogeneous products from the primary zone mix with one another and with the entering cooling air. By the end of the zone the distribution is collapsed to a uni-dimensional profile. To accomplish this mixing process ZINTER calls on Subroutines ZMASS, CHECKK, RUNKUT, MINT, and PRINTS. The function of Subroutines ZMASS and MINT are as before; PRINTS writes the calculated mass mean conditions at the end of each finite length axial combustor segment. Subroutine CHECKK calculates the proportionality constant between the mass flow rate out of an element due to mixing and the total mass flowing into it at a given axial position in the combustor. RUNKUT is employed to obtain the solution to the first order ordinary differential equation between nitric oxide concentration and axial position in the combustors by the Gill variation of the Runge-Kutta numerical integration scheme. In doing so, RUNKUT calls Subroutine DERIV which calculates the rate of nitric oxide formation with respect to axial distance in the combustor intermediate or dilution zone.

In the dilution zone, the flow is uni-dimensional with the gases uniformly mixed across each cross section. To perform and control these calculations GASNOX calls on Subroutine DILUTE. DILUTE in turn calls on Subroutines ZMASS, MINT, RUNKUT, and PRINTS for calculations and printout at specified axial stations in the zone. The only deviation of these subroutines from their previously described functions occurs in ZMASS: since the mixture ratio distribution is collapsed to a flat profile, it omits reference to Subroutine CALCBC.

This concludes the description of the over-all logic structure of Program GASNOX. A modular diagram of GASNOX is provided as Figure 4.

APPENDIX II - COMMON FORTRAN NOMENCLATURE

The following tables contain the COMMON Fortran nomenclature for Program GASNOX. COMMON consists of seven labeled blocks; the nomenclature is arranged in alphabetic order for each block. Singly subscripted arrays are indicated by their respective indices.

I - Element index

J - Incremental station index for the X direction

K - Distribution index

Nomenclature for COMMON/DATA1/

Fortran Symbol	Symbol	Description	Units
AIR(J)	$M_A\}_X$	Combustor airflow at axial station X	gm/sec
ATT(I)	T_i	Adiabatic flame temperature for an element i	deg K
A1	A_1	Exponent in relationship governing collapse of mixture ratio distribution function	
A2	A_2	Factor in relationship defining the rate at which unburned fuel is burned in the intermediate zone	
A3	A_3	Exponent in relationship defining the rate at which unburned fuel is burned in the intermediate zone	
BCON1(I)	$(C_{(s)_i})_e$	Equilibrium mole fraction of carbon for an element i	
BCON2(I)	$(CO_i)_e$	Equilibrium mole fraction of carbon monoxide for an element i	
BCON6(I)	$(NO_i)_e$	Equilibrium mole fraction of nitric oxide for an element i	
BETA		Combustion efficiency in the primary zone	
CH2(I)	$(CH_{2_i})_e$	Equilibrium mole fraction of unburned hydrocarbons exclusive of $C_{(s)}$ and CO for an element i	

Fortran Symbol	Symbol	Description	Units
CN	C_N	Mixing characteristic	
CUMDIS(K)		Value of cumulative normal distribution	
EKS	k_s	Fuel-to-air mass ratio at stoichiometric conditions	
EK1(I)	$(K1)_i$	Ratio of forward reaction rate constants (see Volume 2, Section 2 or Ref 3)	
EK2(I)	$(K2)_i$	Ratio of forward reaction rate constants (see Volume 2, Section 2 or Ref 3)	
FF(I)	F_i	Mixture ratio	
FNOXP	(NO_o)	NO formed in the flame front	ppm
PHIP	$\bar{\phi}_p$	Mean primary zone equivalence ratio accounting for the inefficiency of the primary zone combustion	
PPP	P	Operating pressure	atm
RHO	ρ_i	Density of combustion products for an element	gm/cm^3
RR(J)	R_X	Radius of combustor liner if canannular configuration; equivalent radius of combustor liner if annular configuration	in; cm
R1(I)	$(R_1)_i$	Forward reaction rate for the first kinetic reaction (see Volume 2, Section 2 or Ref 3)	$gm\text{-}mole/cm^3\text{-}sec$
R6(I)	$(R_6)_i$	Forward reaction rate for the sixth kinetic reaction (see Volume 2, Section 2 or Ref 3)	$gm\text{-}mole/cm^3\text{-}sec$
S	S_o	Degree of mixedness in the primary zone	
VP	V_p	Volume of the primary zone	in^3; cm^3
XEND	X_{END}	Length of intermediate zone and dilute zone (combined)	in; cm
XL	X_L	Length of intermediate zone	in; cm
XX(J)	X	Axial position in the combustor	in; cm

Fortran Symbol	Symbol	Description	Units
ZP(K)	Z_p	Limit of integration of cumulative normal distribution	

Nomenclature for COMMON/OUT1/

Fortran Symbol	Symbol	Description	Units
AVCH2D	$[\overline{CH2}^*]_e$	Average equilibrium concentration of unburned hydrocarbons exclusive of $C_{(s)}$ and CO at a given axial station in the combustor	gm/cc
AVCH2F	$\lceil\overline{CH2}\rceil_e$	Average equilibrium concentration of unburned hydrocarbons exclusive of $C_{(s)}$ and CO at a given axial station in the combustor	gm/1000 gm fuel burned
AVCH2G	$[\overline{CH2}]_e$	Average equilibrium concentration of unburned hydrocarbons exclusive of $C_{(s)}$ and CO at a given axial station in the combustor	
AVCH2P	$\{\overline{CH_2}\}_e$	Average equilibrium concentration of unburned hydrocarbons exclusive of $C_{(s)}$ and CO at a given axial station in the combustor	ppm(vol)
AVECOD	$[\overline{CO}^*]_e$	Average equilibrium concentration of CO at a given axial station in the combustor	gm/cc
AVECOF	$\lceil\overline{CO}\rceil_e$	Average equilibrium concentration of CO at a given axial station in the combustor	gm/1000 gm fuel burned
AVECOG	$[\overline{CO}]_e$	Average equilibrium concentration of CO at a given axial station in the combustor	
AVECOP	$\{\overline{CO}\}_e$	Average equilibrium concentration of CO at a given axial station in the combustor	ppm(vol)
AVECSD	$[\overline{C}_s^*]_e$	Average equilibrium concentration of $C_{(s)}$ at a given axial station in the combustor	gm/cc
AVECSF	$\lceil\overline{C}_s\rceil_e$	Average equilibrium concentration of $C_{(s)}$ at a given axial station in the combustor	gm/1000 gm fuel burned
AVECSG	$[\overline{C}_s]_e$	Average equilibrium concentration of $C_{(s)}$ at a given axial station in the combustor	

Fortran Symbol	Symbol	Description	Units
AVECSP	$\{\bar{C}_s\}_e$	Average equilibrium concentration of $C_{(s)}$ at a given axial station in the combustor	ppm(vol)

Nomenclature for COMMON/OUT2/

Fortran Symbol	Symbol	Description	Units
AVENFU	$[\overline{NO}]_{up}$	Average nitric oxide concentration at prior axial station in the combustor	gm/1000 gm fuel burned
AVENOD	$[NO^{*}]$	Average nitric oxide concentration at a given axial station in the combustor	gm/cc
AVENOF	$[\overline{NO}]$	Average nitric oxide concentration at a given axial station in the combustor	gm/1000 gm fuel burned
AVENOG	$[\overline{NO}]$	Average nitric oxide concentration at a given axial station in the combustor	
AVENOP	$\{\overline{NO}\}$	Average nitric oxide concentration at a given axial station in the combustor	ppm(vol)
ILAST		Indicator ILAST = 0 if the nitric oxide chemical reaction is not frozen at a given axial position in the combustor ILAST = 1 if the nitric oxide chemical reaction is frozen at a given axial position in the combustor	
RRO	$(\bar{\rho})_{rr}$	Mean density of combustion products at a given axial station in the combustor	gm/cc

Nomenclature for COMMON/OUT3/

Fortran Symbol	Symbol	Description	Units
AVET	$\bar{T}$	Average temperature of combustion products at a given axial station in the combustor	deg K
FBARD	$\bar{F}$	Mean mixture ratio at a given axial station in the combustor	
IMAX	i_{MAX}	Subscript of mass element with highest equivalence ratio	

Fortran Symbol	Symbol	Description	Units
INDIC		Indicator INDIC = 1 for primary zone INDIC = 2 for intermediate zone type calculation INDIC = 3 for dilution zone type calculation	
LEN		Indicator LEN = 0 if intermediate zone calculations end at X_L LEN = 1 if intermediate zone calculations end at X_{END}	
NO(I)	$[NO_i]$	Nitric oxide concentration for an element i of the distribution function	
PHIBAR	$\bar{\Phi}$	Mean equivalence ratio at a given axial station in the combustor	
RHOBAR	$\bar{\rho}$	Mean density of combustion products at a given axial station in the combustor	gm/cc
TAUBAR	$\bar{\tau}$	Mean residence time in the combustor at a given axial station	sec
TAUDIL	$\bar{\tau}_{DIL}$	Mean residence time in the combustor dilution zone	sec
TAUINT	$\bar{\tau}_{INT}$	Mean residence time in the combustor intermediate zone	sec
VELOC	V	Velocity of combustion products at a given axial station in the combustor	cm/sec
XD	X_D	Axial position (downstream) in the combustor	cm
XU	X_U	Axial position (upstream) in the combustor	cm

Nomenclature for COMMON/OUT4/

Fortran Symbol	Symbol	Description	Units
AIRD	$M_A\|_{X_D}$	Airflow at a given axial station in the combustor	gm/sec

Fortran Symbol	Symbol	Description	Units
ANO	$[\overline{NO}]_{AN}$	Average nitric oxide concentration at a given axial station in the combustor	
AQQ	Q	Measure of the round-off error in the Runge-Kutta integration routine at a given axial station in the combustor	
AREAD	$A]_{X_D}$	Cross-sectional area of combustor at a given axial station in the combustor	cm^2
ASLOPE	$\left(\frac{\partial \dot{m}_A}{\partial X}\right)_{X_D}$	Rate of change of airflow rate in the combustor liner with axial position at a given axial station in the combustor	gm/sec-cm
AVEMW	$\overline{MW}$	Average molecular weight of reaction products at a given axial station in the combustor	gm/gm-mole
CONSNO(I)	$[NO^*_i]_e$	Nitric oxide equilibrium concentration for an element i of the distribution function	
DDM(I)	$(\delta M_i)_D$	Elemental mass flow rate at the downstream limit of integration	gm/sec
DELMD(I)	$(\Delta M_i)_D$	Elemental mass flow rate at the downstream limit of integration	gm/sec
DIFNO(I)		Difference in NO concentrations for successive iterations for an element i of the distribution function	
DMDDA(I)	$(\delta \ddot{m}_A)_i$	Elemental mass flow of gases into control volume due to mixing of the dilution air with previously mixed gases	gm/sec-cm
DMDDM(I)	$(\delta \ddot{m}_M)_i$	Elemental mass flow of gases into control volume due to mixing action of gases already within the combustion liner	gm/sec-cm
DMDDP(I)	$(\delta \ddot{m}')_i$	Total elemental mass flow of gases into control volume due to mixing	gm/sec-cm
DMDDPP(I)	$(\delta \ddot{m}'')_i$	Total elemental mass flow of gases out of control volume due to mixing	gm/sec-cm
DMFFED	$(\dot{M}_f)_{fed}$	Total mass flow of fuel fed to the combustor	gm/sec

Fortran Symbol	Symbol	Description	Units
DMFT	$(\dot{M}_f)_{X_D}$	Total mass flow of combusted fuel at a given axial station in the combustor	gm/sec
DMFUD	$(\dot{M}_{fu})_{X_D}$	Total mass flow of unburned fuel at a given axial station in the combustor	gm/sec
DMFUO	$(\dot{M}_f)_o$	Total mass flow of unburned fuel at the primary zone exit	gm/sec
E(I)	E_i	Proportionality factor between mass flow rate out of an element i due to mixing and the total mass flowing into it	cm^{-1}
EKKD	K_D	Proportionality factor between mass flow rate out of an element due to mixing and the total mass flowing into it	cm^{-1}
FB(I)	$(F_B)_i$	Boundaries between which each mixture ratio value applies	
FPRIME(I)	$(F')_i$	Mixture ratio at entrance to elemental control volume i	
NOEQXD	$[NO_e]_{X_D}$	Mass average nitric oxide equilibrium concentration at a given axial station in the combustor	
NOP(I)	$[NO]_i$	Nitric oxide concentration of the mass flowing into an elemental control volume due to mixing at a given axial station in the combustor	
NOZERO(I)		Indicator NOZERO = 0 if chemical rate of production of NO in an element i is finite NOZERO = 1 if chemical rate of product of NO in an element is zero	
RDOT(I)	$\dot{R}_i$	Elemental rate of change of unburned fuel with axial station in the combustor	gm/sec-cm
RSUBX	R_{X_D}	Combustor radius at a given axial station in the combustor	cm
SIG	σ	Standard deviation of the distribution function at a given axial station in the combustor	
SIGZER	σ_o	Standard deviation of the distribution function in the primary zone of the combustor	

Fortran Symbol	Symbol	Description	Units
SLOPE(I)	$\left[\frac{\partial(\delta \dot{m}_i)}{\partial x}\right]_{x_D}$	Rate of change of elemental mass flow rate with axial position at a given axial station in the combustor	gm/sec-cm
SUEA(I)		Difference in NO concentrations for successive iterations for an element i of the distribution function	
TSLOPE	$\left[\frac{\partial m^*}{\partial x}\right]_{x_D}$	Rate of change of total mass flow rate with axial position at a given axial station in the combustor	gm/sec-cm
UDM(I)	$(\delta \dot{m}_i)_u$	Elemental mass flow rate at the upstream limit of integration	gm/sec

Nomenclature for COMMON /OUT5/

Fortran Symbol	Symbol	Description	Units
MSTARD	M^*_D	Total mass flow at downstream limit of integration	gm/sec
MSTARU	M^*_U	Total mass flow at upstream limit of integration	gm/sec
DILL	$(\dot{r})_{DIL}$	Rate of change of NO concentration with axial position in the combustor dilution zone due to air dilution	cm^{-1}
REAT	$(\dot{r})_{react}$	Rate of change of elemental NO concentration with axial position in the combustor due to chemical reaction	cm^{-1}

APPENDIX III - MAIN ROUTINE GASNOX

The principal function of the main routine is to control the logic of the calculation procedure for the prediction of the nitric oxide emissions from gas turbine combustors. In addition, the main routine reads and writes the input data, sets certain values, and performs many related minor calculations.

The main routine calls Subroutines PRIMRY, ZINTER, and DILUTE. The external input required by the main routine consists of:

ANNR	ANR	APR	ARR	ATT
AXX	BCON1	BCON2	BCON6	BETA
CH2	EKS	EK1	EK2	EQUIV
ERAT	FF	IDATA	IN	KASE
PHI	PHIP	PPP	RHO	R1
R6	S	SET	TAUBAR	TOTAIR
VP	XEND	XL		

The external output provided by the main routine consists of:

ANNR	ANR	APR	ARR	ATT
AXX	BCON1	BCON2	BCON6	BETA
CH2	CUMDIS	EKS	EK1	EK2
EQUIV	ERAT	FF	NOZERO	PHI
PHIP	PPP	RHO	R1	R6
S	SET	TAUBAR	TOTAIR	XEND
XL	VP	ZP		

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols in the main routine which are not part of COMMON. Singly and doubly subscripted arrays are indicated by their respective indices:

I - General index of descriptive data

IJ - Incremental axial station index for combustor air

J - Element index

Fortran Symbol	Symbol	Description	Units
AAR(IJ)	$(\dot{M}_A)_X$	Total mass of airflow into combustor liner at position X (cumulative)	lb/sec
ANNR(IJ)	R_{X_0}	Outer radius of liner at position X; applies only for annular configuration	in
AWR(IJ)	R_{X_I}	Inner radius of liner at position X; applies only for annular configuration	in
APR(IJ)	$(\dot{M}_{A_X})\%$	Per cent of total mass of airflow into combustor liner at position X (cumulative)	
ARR(IJ)	R_X	Radius of liner at position X; applies only for canannular configuration	in
AXX	X	Axial position in the combustor	in
DELAIR	ΔM_{AIR}	Combustor air scaling factor	lb/sec
DEX	ΔX	Combustor length	in
EQUIV	ϕ_p	Mass mean equivalence ratio in the primary zone (before fuel burns)	
ERAT	E_{rat}	Variable for varying $\bar{\phi}_p$ parametrically yet maintaining constant air-to-fuel ratio in the combustor	
IDATA		Number of sets of kinetic, thermodynamic, and equilibrium data and combustor inlet conditions	
IN		Number of sets of combustor dimensions, operating conditions, and primary zone mixedness parameter	
KASE		Number of sets of airflow distribution data	
PHI(J)	ϕ_J	Equivalence ratio of an element j	
SET(I)		Combustor descriptive data	
TOTAIR	M_A	Total mass of air fed into the combustor liner	lb/sec

Analysis Procedure

The step-by-step procedure of the main routine is given below. The Fortran listing of the routine is presented at the conclusion of the step-by-step procedure.

1. Read the input kinetic, thermodynamic, and equilibrium data and the combustor inlet conditions for the case.
2. Set the values of certain parameters.
3. Read the input airflow distribution data.

Step 4 is performed only if the combustor is an annular configuration.

4. Calculate the equivalent can radii as:
   $$R_X = \left[(R_{X_0})^2 - (R_{X_1})^2\right]^{\frac{1}{2}}$$
5. Read the input combustor dimensions, operating conditions, and primary zone mixing parameter.
6. Convert the percentage airflow data to mass flow for each specified axial station by the relationship:
   $$(\dot{M}_A)_X = (M_{A_X})_{\%} * \dot{M}_A/100.0$$
7. Calculate $\bar{\phi}_p$ as
   $$\bar{\phi}_p = \phi_p * S$$
8. Calculate $\tilde{\phi}_p$ as:
   $$\tilde{\phi}_p = \bar{\phi}_p * \bar{E}_{rat}$$
9. Set the values of certain parameters and constants.
10. Write the heading for the airflow distribution data for the case.
11. Calculate the total mass of airflow into the combustor liner for each specified axial station correcting for the effect of E_{rat}.
12. Convert the units of the airflow distribution data to the metric system.
13. Write the input data.
14. Convert the units of the combustor dimensions to the metric system.
15. Using Subroutine PRIMRY, calculate the primary zone exit conditions.

16. Set certain indicators.

Step 17 is performed only if $X_{END} = 0$.

17. Go to step 24.

Step 18 is performed only if $S_o = 0$.

18. Go to step 23.

19. If $X_{END} < X_L$, reset certain indicators.

20. Using Subroutine ZINTER, perform the intermediate zone calculations.

Step 21 is performed only if the chemical rate of formation of nitric oxide is frozen in the intermediate zone.

21. Go to step 23.

Step 22 is performed only if $X_{END} < X_L$.

22. Go to step 24.

23. Using Subroutine DILUTE, perform the dilution zone calculations.

24. If this is the last set of combustor dimensions, operating conditions, and primary zone mixing parameter for the given airflow distribution, continue to step 25. If not, return to step 5.

25. If this is the last set of combustor airflow distribution data for the given kinetic, thermodynamic, and equilibrium data and combustor inlet conditions, continue to step 26. If not, return to step 3.

26. If this is the last set of kinetic, thermodynamic, and equilibrium data and combustor inlet conditions, continue to step 27. If not, return to step 1.

27. Stop.

```
      PROGRAM GASNOX(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION SET(25),PHI(50),AAR(50),AXX(50),APR(50),ARR(50),ANR(50),
     1ANNR(50)
      COMMON/DATA1/AIR(50),RR(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(
     150),ZP(70),CUMDIS(70),VP,RHO(50),BCON6(50),ATT(50),PPP,FNOXP,R1(50
     2),R6(50),EK1(50),EK2(50),A2,A3,XL,CN,BETA,S,PHIP,EKS,XEND,A1
      COMMON/OUT1/AVECSG,AVECOG,AVCH2G,AVECSP,AVECOP,AVCH2P,AVECSD,AVECO
     1D,AVCH2D,AVECSF,AVECOF,AVCH2F
      COMMON/OUT2/AVENOG,AVENOD,AVENOP,AVENOF,AVENFU,RRO,ILAST
      COMMON/OUT3/INDIC,NO(50),AVET TAUBAR,RHOBAR,PHIBAR,IMAX,XD,
     1FBARD,XU,LEN,TAUINT,TAUDIL,VELOC
      COMMON/OUT4/CONCNO(50),DELMD(50),AREAD,ASLOPE,DMFUO,SLOPE(50),TSLO
     1PE,NOP(50),EKKD,DMFT,UDM(50),DDM(50),      FP(50),DMFUD,AIRD,DMFFED
     2,RSUBX,SIG,SIGZER,AVEMW,DMDDA(50),DMDDM(50),DMDDP(50),DMDDPP(50),F
     3PRIME(50),NOEQXD,ANO,AQQ,DIFNO(50),NOZERO(50),RDOT(50),E(50)
      COMMON/OUT5/MSTARD,MSTARU
      DATA(ZP(L),L=1,70)/0.0,0.05,0.10,0.15,0.20,0.25,0.30,0.35,0.40,0.4
     15,0.50,0.55,0.60,0.65,0.70,0.75,0.80,0.85,0.90,0.95,1.0,1.05,1.10,
     21.15,1.20,1.25,1.30,1.35,1.40,1.45,1.50,1.55,1.60,1.65,1.70,1.75,1
     3.80,1.85,1.90,1.95,2.00,2.05,2.10,2.15,2.20,2.25,2.30,2.35,2.40,2.
     445,2.50,2.55,2.60,2.65,2.70,2.75,2.80,2.85,2.90,2.95,3.00,3.05,3.1
     50,3.15,3.20,3.25,3.30,3.35,3.40,3.45/
      DATA(CUMDIS(L),L=1,70)/0.5000,0.5199,0.5398,0.5596,0.5793,0.5987,0
     1.6179,0.6368,0.6554,0.6736,0.6915,0.7088,0.7257,0.7422,0.7580,0.77
     234,0.7881,0.8023,0.8159,0.8289,0.8413,0.8531,0.8643,0.8749,0.8849,
     30.8944,0.9032,0.9115,0.9192,0.9265,0.9332,0.9394,0.9452,0.9505,0.9
     4554,0.9599,0.9641,0.9678,0.9713,0.9744,0.9772,.9798,0.9821,0.9842,
     5.9861,0.9878,0.9893,0.9906,0.9918,0.9929,0.9938,0.9946,0.9953,0.99
     660,0.9965,0.9970,0.9974,0.9978,0.9981,0.9984,0.9987,0.9989,0.9990,
     70.9992,0.9993,0.9994,0.9995,0.9996,0.9997,0.9997/
C****
C**** READ IN AND WRITE OUT THE REQUIRED DATA
C****
      READ(5,50) IDATA
      DO 925  IIK =1,IDATA
      READ(5,400)(SET(I),I=1,15),PPP,SET(16),SET(17),SET(18),SET(19),EKS
  400 FORMAT(12A6/2A6,A2,E15.8,3A6,A4,E15.8)
      DO 600 J = 1,35
      READ(5,450)FF(J),PHI(J),RHO(J),ATT(J),BCON6(J),BCON2(J),BCON1(J),C
     1H2(J),R1(J),R6(J),EK1(J),EK2(J)
      NOZERO(J)=0
      IF(R6(J).EQ.0.0.AND.R1(J).EQ.0.0) NOZERO(J)=1
  600 CONTINUE
  450 FORMAT(6E12.5)
      READ(5,50) KASE
   50 FORMAT(I6)
      DO 900 II = 1,KASE
      DO 300 IJ =1,11
      READ(5,250) AXX(IJ),APR(IJ),ARR(IJ),ANR(IJ),ANNR(IJ)
      XX(IJ) = AXX(IJ)
      RR(IJ) = ARR(IJ)
      IF(RR(IJ).EQ.0.0) RR(IJ) = SQRT(ANNR(IJ)**2.0-ANR(IJ)**2.0)
  300 CONTINUE
  250 FORMAT(5E12.5)
      READ(5,200) IN
  200 FORMAT(I6)
      DO 325 K =1,IN
      READ(5,410) VP,XL,XEND,EQUIV,BETA,TOTAIR,S,ERAT,TAUBAR
      DO 425 IJ=1,11
      AAR(IJ) = APR(IJ)*TOTAIR/100.0
```

```
425 CONTINUE                                                         GAS*0600
    PHIP = EGUIV*BETA                                                GAS*0610
    PHIP=PHIP*ERAT                                                   GAS*0620
    FNOXP = 0.0                                                      GAS*0630
    CN = 5.0                                                         GAS*0640
    A1 = 0.5                                                         GAS*0650
    A2 = 0.5                                                         GAS*0660
    A3 = 1.0                                                         GAS*0670
410 FORMAT(6E12.5/6E12.5)                                            GAS*0680
    DELAIR=AAR(1)*(1.0-1.0/ERAT)                                     GAS*0690
    DEX=XX(11)-XX(1)                                                 GAS*0700
    WRITE(6,100)                                                     GAS*0710
    WRITE(6,775)                                                     GAS*0720
775 FORMAT(///49X,34HCOMBUSTOR AIR FLOW CHARACTERISTICS///)          GAS*0730
    WRITE(6,780)                                                     GAS*0740
780 FORMAT(64X,3HCAN,21X,7HANNULAR)                                  GAS*0750
    WRITE(6,785)                                                     GAS*0760
785 FORMAT(28X,8HDISTANCE,8X,10HPERCENTAGE,9X,6HRADIUS,8X,12HINNER RADGAS*0770
   1IUS,5X,12HOUTER RADIUS)                                          GAS*0780
786 FORMAT(45X,8HAIR FLOW)                                           GAS*0790
    WRITE(6,786)                                                     GAS*0800
    WRITE(6,790)                                                     GAS*0810
790 FORMAT(29X,6HINCHES,28X,6HINCHES,11X,6HINCHES,11X,6HINCHES///)   GAS*0820
    DO 350 IJ=1,11                                                   GAS*0830
    AIR(IJ)=AAR(IJ)-DELAIR*(XX(11)-XX(IJ))/DEX                       GAS*0840
    WRITE(6,825) AXX(IJ),APR(IJ),ARR(IJ),ANR(IJ),ANNR(IJ)            GAS*0850
825 FORMAT(26X,5(E12.5,5X))                                          GAS*0860
    AIR(IJ) = AIR(IJ)*454.                                           GAS*0870
    IF(K.GT.1) GO TO 350                                             GAS*0880
    XX(IJ) = XX(IJ)*2.54                                             GAS*0890
    RR(IJ) = RR(IJ)*2.54                                             GAS*0900
350 CONTINUE                                                         GAS*0910
    WRITE(6,500) K                                                   GAS*0920
500 FORMAT(///58X,11HCASE NO. = ,I6////)                             GAS*0930
    WRITE(6,550)                                                     GAS*0940
550 FORMAT(///48X,35HCUMULATIVE NORMAL DISTRIBUTION DATA////)        GAS*0950
    WRITE(6,115)                                                     GAS*0960
115 FORMAT(14X,2HZP,3X,6HCUMDIS,5X,2HZP,3X,6HCUMDIS,5X,2HZP,3X,6HCUMDIGAS*0970
   1S,5X,2HZP,3X,6HCUMDIS,5X,2HZP,3X,6HCUMDIS,5X,2HZP,3X,6HCUMDIS,5X,2GAS*0980
   2HZP,3X,6HCUMDIS///)                                              GAS*0990
    DO 120 L=1,10                                                    GAS*1000
    WRITE(6,110) ZP(L),CUMDIS(L),ZP(L+10),CUMDIS(L+10),ZP(L+20),CUMDISGAS*1010
   1(L+20),ZP(L+30),CUMDIS(L+30),ZP(L+40),CUMDIS(L+40),ZP(L+50),CUMDISGAS*1020
   2(L+50),ZP(L+60),CUMDIS(L+60)                                     GAS*1030
110 FORMAT(12X,7(F4.2,3X,F6.4,3X))                                   GAS*1040
120 CONTINUE                                                         GAS*1050
    WRITE(6,100)                                                     GAS*1060
    WRITE(6,650)                                                     GAS*1070
650 FORMAT(///58X,16HEQUILIBRIUM DATA///)                            GAS*1080
    WRITE(6,675)(SET(I),I=1,15),PPP,SET(16),SET(17),SET(18),SET(19),EKGAS*1090
   1S                                                                GAS*1100
675 FORMAT(1X,14A6,A2,E15.8/33X,3A6,A4,E15.8///)                     GAS*1110
    WRITE(6,680)                                                     GAS*1120
680 FORMAT(1X,123HTHE FOLLOWING DATA TABLE CONTAINS THE THERMODYNAMIC GAS*1130
   1PROPERTIES,KINETIC RATE CONSTANTS,AND EQUILIBRIUM COMPOSITIONS FORGAS*1140
   2 EACH/1X,124HPRESCRIBED EQUIVALENCE RATIO.  FOR EACH ELEMENT THESEGAS*1150
   3 PROPERTIES ARE,IN ORDER OF PRINTING...MIXTURE RATIO,EQUIVALENCE RGAS*1160
   4ATIO,/1X,119HDENSITY,ADIABATIC FLAME TEMPERATURE,NO,CO,C(S),AND CHGAS*1170
   52(UNBURNED HYDROCARBONS) EQUILIBRIUM MOLE FRACTION,AND THE KINETICGAS*1180
   6/1X,27HPARAMETERS R1,R6,K1,AND K2.//)                            GAS*1190
```

```
      WRITE(6,690)
  690 FORMAT(24X,7HELEMENT/)
      DO 750 J =1,35
      WRITE(6,700) J,FF(J),PHI(J),RHO(J),ATT(J),BCON6(J),BCON2(J),BCON1(
     1J),CH2(J),R1(J),R6(J),EK1(J),EK2(J)
  700 FORMAT(26X,I2,3X,6E12.5/31X,6E12.5)
  750 CONTINUE
      WRITE(6,100)
      WRITE(6,850)
  850 FORMAT(///51X,31HTHE REST OF THE INPUT VARIABLES///)
      WRITE(6,851) VP
  851 FORMAT(10X,34HTHE VOLUME OF THE PRIMARY ZONE IS ,E12.5,7H CU.IN.//
     1)
      WRITE(6,852) XL
  852 FORMAT(10X,39HTHE LENGTH OF THE INTERMEDIATE ZONE IS ,E12.5,4H IN.
     1//)
      WRITE(6,853) XEND
  853 FORMAT(10X,67HTHE LENGTH OF THE INTERMEDIATE ZONE AND DILUTION ZON
     1E(COMBINED) IS ,E12.5,4H IN.//)
      WRITE(6,854) EQUIV
  854 FORMAT(10X,43HTHE MEAN PRIMARY ZONE EQUIVALENCE RATIO IS ,E12.5//)
      WRITE(6,855) BETA
  855 FORMAT(10X,49HTHE COMBUSTION EFFICIENCY IN THE PRIMARY ZONE IS ,E1
     12.5//)
      WRITE(6,856) TOTAIR
  856 FORMAT(10X,48HTHE TOTAL MASS OF AIR FED INTO THE COMBUSTOR IS ,E12
     1.5,9H LB./SEC.//)
      WRITE(6,857) S
  857 FORMAT(10X,27HTHE DEGREE OF MIXEDNESS IS ,E12.5//)
      WRITE(6,858) ERAT
  858 FORMAT(10X,7HERAT = ,E12.5//)
      WRITE(6,859) TAUBAR
  859 FORMAT(10X,105HTHE MEAN PRIMARY ZONE RESIDENCE TIME(ONLY APPLIES I
     1F THE VOLUME OF THE PRIMARY ZONE IS ZERO IN INPUT) IS ,E12.5,5H SE
     2C.)
      VP = VP*2.54*2.54*2.54
      XL = XL*2.54
      XEND = XEND*2.54
  100 FORMAT(1H1)
C****
C**** PERFORM PRIMARY ZONE CALCULATIONS
C****
      CALL PRIMRY
C****
C**** PERFORM INTERMEDIATE ZONE CALCULATIONS
C****
      LEN = 0
      IF(XEND.EQ.0.0) GO TO 1000
      IF(S.EQ.0.0) GO TO 950
      IF(XEND.LT.XL) LEN = 1
      CALL ZINTER
C****
C**** PERFORM DILUTION ZONE CALCULATIONS
C****
      IF(ILAST.EQ.1) GO TO 950
      IF(LEN.EQ.1) GO TO 1000
  950 CALL DILUTE
 1000 CONTINUE
  325 CONTINUE
  900 CONTINUE
```

```
925 CONTINUE                                                        GAS*1800
    STOP                                                            GAS*1810
    END                                                             GAS*1820
```

APPENDIX IV - SUBROUTINE PRIMRY

The function of Subroutine PRIMRY is to calculate the nitric oxide emissions at the primary zone exit of a gas turbine combustor.

Subroutine PRIMRY is called by the main routine (GASNOX); it, in turn, calls Subroutines PRCALC, ZMASS, and PRINTS. The subroutine does not require external input but does provide external output. Internal input and output are transmitted through COMMON. The internal input consists of:

ATT	BCON1	BCON2	BCON6	CH2
FNOXP	PHIP	PPP	RHO	S
TAUBAR	VP			

The internal output consists of:

ANO	AVCH2D	AVCH2F	AVCH2G	AVCH2P
AVECOD	AVECOF	AVECOG	AVECOP	AVECSD
AVECSF	AVECSG	AVECSP	AVEMW	AVENOD
AVENOF	AVENOG	AVENOP	AVET	CONGNO
FNOXG	INDIC	PHIBAR	RHOBAR	TAUBAR
VELOC	XD	XU		

The external output consists of:

FELD	I	QQNO	QSUMNO

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols used in Subroutine PRIMRY which are not included in COMMON.

Fortran Symbol	Symbol	Description	Units
CH2AV	$(\overline{CH_2})_e$	Average equilibrium mole fraction of unburned hydrocarbons exclusive of $C_{(s)}$ and CO in the primary zone	
COAV	$(\overline{CO})_e$	Average equilibrium mole fraction of CO in the primary zone	
CSAV	$(\overline{C_{(s)}})_e$	Average equilibrium mole fraction of $C_{(s)}$ in the primary zone	

Fortran Symbol	Symbol	Description	Units
DELX	δx	Increment of the combustor length across which the solution is generated	cm
FELD(I)	$(M_{frac})_i$	Element i mass fraction	
FNOXG	$[NO_o]$	NO formed in the flame front (mass fraction)	
I	i	Index of the element	
NPRINT		Indicator NPRINT = 0 if intermediate output is not requested by the user NPRINT = 1 if intermediate output is requested by the user	
QQNO(I)	$[NO_i]$	Nitric oxide concentration in the element i	ppm(vol)
QSUMNO(I)	$\Sigma NO{-}\dot{m}$	The cumulative sum of the NO formed up to and including the element i	lb/sec
SUMCHI	$\Sigma CH{-}\dot{m}$	Sum of the elemental mass flow rates times their respective unburned hydrocarbon (exclusive of CO and $C_{(s)}$) equilibrium mole fractions	gm/sec
SUMCOI	$\Sigma CO{-}\dot{m}$	Sum of the elemental mass flow rates times their respective CO equilibrium mole fractions	gm/sec
SUMCSI	$\Sigma C_{(s)}{-}\dot{m}$	Sum of the elemental mass flow rates times their respective $C_{(s)}$ equilibrium mole fractions	gm/sec
SUMNOI	$\Sigma NO{-}\dot{m}$	Sum of the elemental mass flow rates times their respective NO mass fractions	gm/sec
SUMTI	$\Sigma T{-}\dot{m}$	Sum of the elemental mass flow rates times their respective adiabatic flame temperatures	gm-deg K/sec

Analysis Procedure

The step-by-step procedure of Subroutine PRIMRY is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Convert (NO_o) to $[NO_o]$ by
   $[NO_o] = (NO_o)*10^{-6}*\frac{30.0}{28.0}$
2. Set the values of X_U, X_D, and ΔX as:
   $X_U = 0.0$
   $X_D = 0.0$
   $\Delta X = 0.0$
3. Using Subroutine ZMASS, calculate the mass in each element, the mean mixture ratio, the airflow, and the total mass flow.
4. Calculate $\bar{\rho}$ as:

$$\bar{\rho} = \sum_{i=1}^{i_{MAX}} \rho_i*(\Delta \dot{M}_i)_D/\dot{M}_D^* \qquad S_0 \neq 0$$

$$\bar{\rho} = \rho_{i_{MAX}} \qquad S_0 = 0$$

Step 5 is performed if $V_p \neq 0.0$

5. Go to step 8.
6. Calculate V_p as:

$$V_P = \frac{\bar{\tau}*\dot{M}_D^*}{\bar{\rho}}$$

7. Go to step 9.
8. Calculate $\bar{\tau}$ as:

$$\bar{\tau} = \frac{V_P*\bar{\rho}}{\dot{M}_D^*}$$

9. Calculate $[NO_i]_e$ as:

$$[NO_i]_e = \sum_{i=1}^{i_{MAX}} \frac{(NO_i)_e*30.0}{\rho_i*T_i*82.057/P} \qquad S_0 \neq 0$$

$$[NO_i]_e = \frac{(NO_{i_{MAX}})_e*30.0}{\rho_{i_{MAX}}*T_{i_{MAX}}*82.057/P} \qquad S_0 = 0$$

10. Using Subroutine PRCALC, calculate the NO concentration in each element in the distribution.

Step 11 is performed only if intermediate output is requested by the user.

11. Write the heading identifying the primary zone elemental exit conditions.

12. For each element in which m_i is non-zero, calculate $\Sigma NO\text{-}m$, $\Sigma C_{(s)}\text{-}m$, $\Sigma CO\text{-}m$, $\Sigma CH\text{-}m$, $\Sigma T\text{-}m$, and $(M_{frac})_i$ as:

$$\Sigma NO\text{-}m = \sum_{i=1}^{imax} [NO_i] (\Delta M_i)_D$$

$$\Sigma C_{(s)}\text{-}m = \sum_{i=1}^{imax} (C_{(s)i})_e (\Delta M_i)_D$$

$$\Sigma CO\text{-}m = \sum_{i=1}^{imax} (CO_i)_e (\Delta M_i)_D$$

$$\Sigma CH\text{-}m = \sum_{i=1}^{imax} (CH_{2i})_e (\Delta M_i)_D$$

$$\Sigma T\text{-}m = \sum_{i=1}^{imax} T_i (\Delta M_i)_D$$

$$(M_{frac})_i = (\Delta M_i)_D / M^*_D$$

Steps 13-14 are performed only if intermediate output is requested by the user.

13. Convert the units of $\Sigma NO\text{-}m$ from gm/sec to lb/sec.

14. Convert the units of $[NO_i]$ from mass fraction to ppm(vol) - $\frac{\text{gm-mole}}{\text{gm}}$

15. Calculate $[\overline{NO}]$, $\overline{T}$, and $\overline{MW}$ as:

$$[\overline{NO}] = \Sigma NO\text{-}m / M^*_D$$

$$\overline{T} = \Sigma T\text{-}m / M^*_D$$

$$\overline{MW} = \overline{\rho} * \overline{T} * 82.057 / P$$

Steps 16-17 are performed only if intermediate output is requested by the user.

16. Convert the units of $[NO_i]$ from ppm(vol) - $\frac{\text{gm-mole}}{\text{gm}}$ to ppm(vol).

17. For each element in the distribution, write the element mass fraction, the nitric oxide concentration (ppm-vol),

the cumulative sum of the NO formed up to and including the element, and the element number.

18. Calculate $\bar{\phi}$ as

$$\bar{\phi} = \bar{\phi}_{P}$$

19. Calculate V as

$$V = \dot{m}_D^* / \bar{\rho} * A |_{x_D}$$

20. Calculate $\{\overline{NO}\}$, $[\overline{NO}^*]$, $\lceil \overline{NO} \rfloor$ as:

$$\{\overline{NO}\} = [\overline{NO}] * 10^6 * \overline{MW} / 30.0$$

$$[\overline{NO}^*] = [\overline{NO}] * \bar{\rho}$$

$$\lceil \overline{NO} \rfloor = [\overline{NO}] * \dot{m}_D^* * 1000 / (\dot{M}_F)_{x_D}$$

21. Calculate $(\bar{C}_{(s)})_e$, $(\overline{CO})_e$, and $(\overline{CH_2})_e$ as:

$$(\bar{C}_{(s)})_e = \Sigma C_{(s)}\text{-}m / \dot{m}_D^*$$

$$(\overline{CO})_e = \Sigma CO\text{-}m / \dot{m}_D^*$$

$$(\overline{CH_2})_e = \Sigma CH_2\text{-}m / \dot{m}_D^*$$

22. Calculate $[\bar{C}_{(s)}]_e$, $[\overline{CO}]_e$, and $[\overline{CH_2}]_e$ as:

$$[\bar{C}_{(s)}]_e = (\bar{C}_{(s)})_e * 12 / \overline{MW}$$

$$[\overline{CO}]_e = (\overline{CO})_e * 28 / \overline{MW}$$

$$[\overline{CH_2}]_e = (\overline{CH_2})_e * 14 / \overline{MW}$$

23. Calculate $\{\bar{C}_{(s)}\}_e$, $\{\overline{CO}\}_e$, and $\{\overline{CH_2}\}_e$ as:

$$\{\bar{C}_{(s)}\}_e = [\bar{C}_{(s)}]_e * 10^6 * \overline{MW} / 12$$

$$\{\overline{CO}\}_e = [\overline{CO}]_e * 10^6 * \overline{MW} / 28$$

$$\{\overline{CH_2}\}_e = [\overline{CH_2}]_e * 10^6 * \overline{MW} / 14$$

24. Calculate $[\bar{C}_{(s)}^*]_e$, $[\overline{CO}^*]_e$, and $[\overline{CH_2}^*]_e$ as:

$$[\bar{C}_{(s)}^*]_e = [\bar{C}_{(s)}]_e * \bar{\rho}$$

$$[\overline{CO}^*]_e = [\overline{CO}]_e * \bar{\rho}$$

$$[\overline{CH_2}^*]_e = [\overline{CH_2}]_e * \bar{\rho}$$

25. Calculate $\{\bar{C}_{(s)}\}_e$, $\{\overline{CO}\}_e$, and $\{\overline{CH_2}\}_e$ as:

$$\{\bar{C}_{(s)}\}_e = [\bar{C}_{(s)}]_e * \dot{M}^*_D * 1000/(\dot{M}_f)_{x_D}$$

$$\{\overline{CO}\}_e = [\overline{CO}]_e * \dot{M}^*_D * 1000/(\dot{M}_f)_{x_D}$$

$$\{\overline{CH_2}\}_e = [\overline{CH_2}]_e * \dot{M}^*_D * 1000/(\dot{M}_f)_{x_D}$$

26. Using Subroutine PRINTS, write the output for the primary zone.

27. Return.

```
      SUBROUTINE PRIMRY
      REAL NO
      REAL MSTARD,MSTARU
      DIMENSION QQNO(50),QSUMNO(50),FELD(50)
      COMMON/DATA1/AIR(50),RR(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(
     150),ZP(70),CUMDIS(70),VP,RHO(50),BCON6(50),ATT(50),PPP,FNOXP,R1(50
     2),R6(50),EK1(50),EK2(50),A2,A3,XL,CN,BETA,S,PHIP,EKS,XEND,A1
      COMMON/OUT1/AVECSG,AVECOG,AVCH2G,AVECSP,AVECOP,AVCH2P,AVECSD,AVECO
     1D,AVCH2D,AVECSF,AVECOF,AVCH2F
      COMMON/OUT2/AVENOG,AVENOD,AVENOP,AVENOF,AVENFU,RRO,ILAST
      COMMON/OUT3/INDIC,NO(50),AVET,TAUBAR,RHOBAR,PHIBAR,IMAX,XD,
     1FBARD,XU,LEN,TAUINT,TAUDIL,VELOC
      COMMON/OUT4/CONGNO(50),DELMD(50),AREAD,ASLOPE,DMFUO,SLOPE(50),TSLO
     1PE,NOP(50),EKKD,DMFT,UDM(50),DDM(50),     FB(50),DMFUD,AIRD,DMFFED
     2,RSUBX,SIG,SIGZER,AVEMW,DMDDA(50),DMUDM(50),DMDDP(50),DMDDPP(50),F
     3PRIME(50),NOEQXD,ANO,AQQ,DIFNO(50),NOZERO(50),ROOT(50),E(50)
      COMMON/OUT5/MSTARD,MSTARU
      NPRINT=1
      INDIC = 1
C****
C**** CONVERT FLAME NO UNITS (NOTE...MEAN MW TAKEN AS 28.0)
C****
      FNOXG=FNOXP*1.0E-06*(30.0/28.0)
C****
C**** CALCULATE MASS IN EACH ELEMENT
C****
      XU = 0.0
      XD = 0.0
      DELX = 0.0
      CALL ZMASS(DELX)
      WRITE(6,100)
C****
C**** CALCULATE AVERAGE RHO AND TAU
C****
      RHOBAR = 0.0
      DO 1000 I = 1,IMAX
      IF(S.EQ.0.0.AND.I.LT.IMAX) GO TO 1000
      RHOBAR = RHOBAR+RHO(I)*DELMD(I)/MSTARD
 1000 CONTINUE
      IF(VP.NE.0.0) GO TO 1025
      VP=TAUBAR*MSTARD/RHOBAR
      GO TO 1050
 1025 TAUBAR=(VP*RHOBAR/MSTARD)
 1050 CONTINUE
C****
C**** DO NO CALCULATIONS
C****
      SUMNOI = 0.0
      SUMTI = 0.0
      SUMCSI = 0.0
      SUMCOI = 0.0
      SUMCHI = 0.0
      DO 2000 I = 1,IMAX
      IF(S.EQ.0.0.AND.I.LT.IMAX) GO TO 2000
      CONGNO(I) = BCON6(I)*30.0/(RHO(I)*ATT(I)*82.057/PPP)
 2000 CONTINUE
      CALL PRCALC(FNOXG)
      IF(NPRINT.EQ.0) GO TO 2500
      WRITE(6,9987)
 9987 FORMAT(///,52X,28HPRIMARY ZONE EXIT CONDITIONS)
```

```
      WRITE(6,9988)
 9988 FORMAT(///,46X,4HMASS,9X,2HNO,8X,8HTOTAL NO,7X,7HELEMENT)
      WRITE(6,9989)
 9989 FORMAT(44X,8HFRACTION,5X,8HPPM(VOL),5X,6HLB/SEC,10X,3HNO.,/)
 2500 CONTINUE
      DO 3000 I =1,IMAX
      IF(DELMD(I).EQ.0.0) GO TO 3000
      SUMNOI = SUMNOI+NO(I)*DELMD(I)
      SUMCSI = SUMCSI+BCON1(I)*DELMD(I)
      SUMCOI = SUMCOI + BCON2(I)*DELMD(I)
      SUMCHI = SUMCHI+CH2(I)*DELMD(I)
      SUMTI = SUMTI+ATT(I)*DELMD(I)
      FELD(I) = DELMD(I)/MSTARD
      IF(NPRINT.EQ.0) GO TO 3000
      QSUMNO(I) = SUMNOI/454.0
      QQNO(I) = NO(I)*1.0E+06/30.0
 3000 CONTINUE
      AVENOG = SUMNOI/MSTARD
      ANO = AVENOG
      AVET = SUMTI/MSTARD
      AVEMW = RHOBAR*AVET*82.057/PPP
      IF(NPRINT.EQ.0)  GO TO 3200
      DO 3100 I =1,IMAX
      QQNO(I) = QQNO(I)*AVEMW
      WRITE(6,9990) FELD(I),QQNO(I),QSUMNO(I),I
 9990 FORMAT(42X,3E12.5,7X,I3)
 3100 CONTINUE
 3200 CONTINUE
C****
C**** CALCULATE VELOCITY AND PHIBAR
C****
      PHIBAR = PHIP
      VELOC = MSTARD/(RHOBAR*AREAD)
      AVENOP=AVENOG*1.0E+06*AVEMW/30.0
      AVENOD = AVENOG*RHOBAR
      AVENOF = AVENOG*MSTARD*1000./DMFT
      CSAV = SUMCSI/MSTARD
      COAV = SUMCOI/MSTARD
      CH2AV = SUMCHI/MSTARD
      AVECSG = CSAV*12.0/AVEMW
      AVECOG = COAV*28.0/AVEMW
      AVCH2G = CH2AV*14.0/AVEMW
      AVECSP=AVECSG*1.0E+06*AVEMW/12.0
      AVECOP=AVECOG*1.0E+06*AVEMW/28.0
      AVCH2P=AVCH2G*1.0E+06*AVEMW/14.0
      AVECSD = AVECSG*RHOBAR
      AVECOD = AVECOG*RHOBAR
      AVCH2D = AVCH2G*RHOBAR
      AVECSF=AVECSG*MSTARD*1000.0/DMFT
      AVECOF = AVECOG*MSTARD*1000./DMFT
      AVCH2F = AVCH2G*MSTARD*1000./DMFT
      CALL PRINTS
  100 FORMAT(1H1)
      RETURN
      END
```

APPENDIX V - SUBROUTINE ZINTER

The function of Subroutine ZINTER is to calculate the concentration of nitric oxide at specified axial stations, and at the exit, of the intermediate zone of a gas turbine combustor.

Subroutine ZINTER is called by the main routine (GASNO): it, in turn, calls Subroutines MINT, CHECKK, RUNKUT, ZMASS, and PRINTS. The subroutine does not require external input but does provide external output. Internal input and output are transmitted through COMMON. The internal input consists of:

ATT	BCON1	BCON2	BCON6	CH2
CN	CONGNO	EKS	EK1	EK2
FF	LEN	NO	NOZERO	PPP
RHO	RSUBX	R1	R6	TAUBAR
XD	XEND	XL		

The internal output consists of:

ANO	AQQ	AVCH2D	AVCH2F	AVCH2G
AVCH2P	AVECOD	AVECOF	AVECOG	AVECOP
AVECSD	AVECSF	AVECSG	AVECSP	AVEMW
AVENFU	AVENOD	AVENOF	AVENOG	AVENOP
AVET	CONGNO	DMDDA	DMDDM	DMDDP
DMDDPP	EKKD	ILAST	INDIC	LEN
NO	NOP	PHIBAR	RHOBAR	RRO
TAUBAR	TAUINT	VELOC	XD	XU

The external output consists of:

AVNO	AVRHO	DDFNO	E	IIE
J	N	XD		

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols used in Subroutine ZINTER which are not included in COMMON:

Fortran Symbol	Symbol	Description	Units
AVNO(J)	NO_j	Mass average nitric oxide concentration for a given iteration j at the end of each major step in the combustor	

Fortran Symbol	Symbol	Description	Units
AVRHO(J)	$\tilde{\rho}_j$	Mass average density of the combustion products for a given iteration j at the end of each major step in the combustor	gm/cc
AVVNO	rat_1	Ratio of total nitric oxide mixing out of the elements to the total mass mixing into the elements	
AVVNOG	$\overline{NO}$	Mass average nitric oxide concentration for a given iteration at a given axial step in the combustor	
CH2AV	$(\overline{CH}_2)_e$	Mass average equilibrium mole fraction of unburned hydrocarbons (exclusive of $C_{(s)}$ and CO) at a given axial station in the combustor	
CNOLST	$[NO]_{IK}$	Nitric oxide equilibrium concentration for the last incremental step in the intermediate zone	
COAV	$(\overline{CO})_e$	Mass average equilibrium mole fraction of carbon monoxide at a given axial station in the combustor	
CSAV	$(\overline{C}_s)_e$	Mass average equilibrium mole fraction of $C_{(s)}$ at a given axial station in the combustor	
DDFNO	$[\Delta NO]$	Measure of difference in the calculated NO levels after successive iterations at a given axial station in the combustor	
DELTAX	ΔX	Integration step size (major) in the intermediate zone	cm
DELX	δX	Increment of the combustor length across which the solution is generated	cm
DIFNO	$[\Delta NO]$	Measure of difference in the calculated NO levels after successive iterations at a given axial station in the combustor	
DUMMY	$[NO]_{DUM}$	Dummy variable	
EK*	k_e	Constant - equal to 0.05	
EK1LST	$(K_1)_{LST}$	Ratio of forward reaction rate constants for the last step in the intermediate zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)	

*Variable initialized but not used in subroutine

Fortran Symbol	Symbol	Description	Units
EK2LST	$(K_2)_{LST}$	Ratio of forward reaction rate constants for the last step in the intermediate zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)	
EN	N	Proportionality constant between ΔX and δX	
FFF	F	Mean mixture ratio for the last step in the intermediate zone	
FURAT	$[\Delta \overline{NO}]_{\Delta x}$	Measure of change in NO concentration for successive steps in the combustor	
GNOMI	$[NO]_{gm}$	Nitric oxide content of an element i at a given axial station in the combustor	gm
IENDZ		Indicator IENDZ = 0 for all except the last major integration step in the intermediate zone IENDZ = 1 for the last major integration step in the intermediate zone	
II	II	Integration increment index	
IIE	I_{ie}	Counter of number of iterations attempting to satisfy ε_i criteria	
J	J	Number of iterations for each major axial step in the combustor	
K	K	Number of iterations for each major axial step in the combustor	
KON(I)*		Index KON(I) = 0 if integration for the element has not converged KON(I) = 1 if integration for the element has converged	
LSGN		Indicator LSGN = 1 if intermediate zone and not the last step in the zone LSGN = 2 if intermediate zone and the last step in the zone LSGN = 3 if dilution zone	

*Variable initialized but not used in subroutine

Fortran Symbol	Symbol	Description	Units
N	N	Proportiona :y constant between ΔX and δX	
NOAVGS**	$[NO]_{spec}$	Nitric oxide concentration of the last element in the array	
NONO(I)	$[NO_i]_{NO}$	Dummy variable	
NOSTAR**	$[NO^*]$	Nitric oxide concentration of the combustion products before air addition at a given axial station in the combustor	
NPRINT		Indicator NPRINT = 0 if intermediate output is not requested by the user NPRINT = 1 if intermediate output is requested by the user	
OUTNO	$[NO]_{0-1}$	Total nitric oxide mixing out of the elements at a given axial station in the combusto. intermediate zone	gm/sec-cm
OUTNO2	$[NO]_{0-2}$	Total nitric oxide at a given upstream axial station in the combustor intermediate zone	gm/sec
PINO	M_{in}	Total mass mixing into the elements at a given axial station in the combustor	gm/sec-cm
Q(I)	q_i	Measure of the round-off error for the element i at a given axial station in the combustor	
QQ(I)	qq_i	Measure of the round-off error for the element i at a given axial station in the combustor	
RHOLST	ρ_{LST}	Density of combustion products for the last step in the intermediate zone at the mean mixture ratio	gm/cm^3
RHOMI	$D\rho$	Dummy variable	gm^2/cm^3
R1LST	$(R_1)_{LST}$	Forward reaction rate for the first kinetic reaction for the last step in the intermediate zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)	gm-mole/cm^3-sec

**Variable set real but not used in subroutine.

Fortran Symbol	Symbol	Description	Units
R6LST	$(R_6)_{LST}$	Forward reaction rate for the sixth kinetic reaction for the last step in the intermediate zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)	gm-mole/cm^3-sec
STEPS	n_{step}	Number of remaining integration steps before end of intermediate zone	
STORE1		Dummy variable	gm-mole/cm^3-sec
STORE2		Dummy variable	gm-mole/cm^3-sec
STORE3		Dummy variable	
STORE4		Dummy variable	
STORE5		Dummy variable	
STORE6		Dummy variable	deg K
STORE7		Dummy variable	gm/cm^3
SUMNOI	$\Sigma_{NO/i}$	Summation of the total nitric oxide present at a given axial location in the intermediate zone	gm
SUM1(J)	$(\Sigma_1)_j$	Dummy variable	gm^2/cm^3
SUM2(J)	$(\Sigma_2)_j$	Summation of the total nitric oxide present at a given axial location in the intermediate zone at the jth iteration at that point	gm
TAU	$\bar{\tau}_{inc}$	Incremental residence time	sec
TTLAST	T_{LST}	Adiabatic flame temperature for the last step in the intermediate zone at the mean mixture ratio	deg K
XI	X_I	Integrated length of intermediate zone	cm
XXX	X_{XX}	Axial position in the combustor	cm
XXXX	X_{XXX}	Distance between upstream end of integration interval and end of intermediate zone	cm
YNOLST	$(NO_e)_{LST}$	Equilibrium mole fraction of NO for the last step in the intermediate zone at the mean mixture ratio	

<u>Analysis Procedure</u>

The step-by-step procedure of Subroutine ZINTER is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Initialize indicators.
2. Initialize $\lfloor \bar{NO} \rceil_{UP}$ as:

$$\lfloor \bar{NO} \rceil_{UP} = 0$$

3. Set k_e as:

   $k_e = 0.05$
4. Calculate X_U as

   $X_U = X_D$
5. Initialize $\bar{\bar{T}}_{INT}$ as:

$$\bar{\bar{T}}_{INT} = 0$$

Step 6 is performed for each potential array element satisfying the criteria $1 \leq i \leq 50$.

6. Initialize q_i as:

   $q_i = 1.0 \times 10^{-15}$
7. Calculate ΔX as:

$$\Delta X = 0.1 * R_{X_D}$$

8. Calculate X_I as:

   $X_I = X_L - X_U$ if intermediate zone calculations end at X_L

   $X_I = X_{END} - X_U$ if intermediate zone calculations end at X_{END}

Step 9 is performed only if $\Delta X \leq X_I$

9. Go to step 12.
10. Recalculate ΔX as:

$$\Delta X = X_I$$

11. Reset the indicator to indicate that this is the last major integration step in the intermediate zone.

Steps 12 and 13 are performed for each potential array element satisfying the criteria: $1 \leq i \leq 50$

12. Calculate $[NO_i]_{NO}$ and qq_i as

$$[NO_i]_{NO} = [NO_i]$$
$$qq_i = q_i$$

13. Initialize convergence indicators.

Step 14 is performed for each potential integration iteration satisfying the criteria $1 \leq J \leq 6$

14. Initialize $(\varepsilon_1)_j$ and $(\varepsilon_2)_j$ as:

$$(\varepsilon_1)_j = 0$$
$$(\varepsilon_2)_j = 0$$

15. Set X_{XX} equal to X_D.

16. Set J and N as:

J = 1

N = 5

Step 17 is performed only if J = 1.

17. Go to step 21.

18. Calculate X_U and X_D as:

$$X_U = X_{XX}$$
$$X_D = X_U$$

19. Using Subroutine ZMASS, calculate the elemental and over-all mass flow rates, the mean mixture ratio, and the airflow rate at X_D.

Step 20 is performed for each element in the array satisfying the criteria $1 \leq i \leq i_{MAX}$

20. Calculate $[NO_i]$ and q_i as:

$$[NO_i] = [NO_i]_{NO}$$
$$q_i = qq_i$$

21. Calculate δX as:

$$\delta X = \Delta X / N$$

22. Calculate K_D and $\overline{NO}$ as:

$$K_D = C_N / X_L$$
$$\overline{NO} = [\overline{NO}]$$

23. Set II = 1.

24. Initialize $[NO]_{O-1}$, $[NO]_{O-2}$ and $[NO]_{P-1N}$ as:

$$[NO]_{O-1} = 0$$
$$[NO]_{O-2} = 0$$
$$[NO]_{P-1N} = 0$$

25. Calculate X_D as:

$$X_D = X_U + \delta X$$

Step 26 is performed only if II = N and if this is the last major integration step in the intermediate zone.

26. Go to step 100.
27. Using Subroutine ZMASS, calculate the elemental and over-all mass flow rates, the mean mixture ratio, and the airflow rate at X_D.
28. Using Subroutine CHECKK, calculate the proportionality constant between the mass flow rate out of an element due to mixing and the total mass flowing into it.
29. Set i = 1.
30. Initialize I_{ie} as:

$$I_{ie} = 0$$

Step 31 is performed only if $\left[\frac{\partial(\delta m_i)}{\partial x}\right]_{X_D} < 0$ and if $(\delta m_i)_D = 0$.

31. Calculate $[NO]_{O-2}$ as:

$$[NO]_{O-2} = [NO]_{O-2} + (\delta m_i)_U * [NO_i]$$

Step 32 is performed only if $(\delta m_i)_D = 0$.

32. Go to step 44.
33. Calculate $(\delta \ddot{m}_A)_i$ as:

$$(\delta \ddot{m}_A)_i = (\delta m_i)_U * \left(\frac{\partial M_A}{\partial x}\right)_{X_D} / M_U^*$$

34. Calculate $(\delta \ddot{m}')_i$, $(\delta \ddot{m}_m)_i$ and $(\delta \ddot{m}'')_i$ as:

$$(\delta \ddot{m}')_i = \left[\frac{\partial(\delta m_i)}{\partial x}\right]_{X_D} + E_i * (\delta m_i)_U - \dot{R}_i$$
$$(\delta \ddot{m}_m)_i = (\delta \ddot{m}')_i - (\delta \ddot{m}_A)_i$$
$$(\delta \ddot{m}'')_i = E_i * (\delta m_i)_U$$

Step 35 is performed only if $(\delta \dot{m}''_m)_i > 0$

35. Go to step 43.

36. Calculate E_i as:

$E_i = 2E_i$

Step 37 is performed only if $E_i = 0$.

37. Calculate E_i as:

$E_i = 0.02$

38. Calculate I_{ie} as:

$I_{ie} = I_{ie} + 1$

Step 39 is performed only if $I_{ie} < 40$.

39. Go to step 34.

40. Write I_{ie} and E_i.

41. Reset the appropriate indicator to indicate that intermediate zone calculations end at X_{END}.

42. Go to step 125.

43. Calculate $[NO]_{O-1}$ and M_{IN} as:

$$[NO]_{O-1} = [NO]_{O-1} + (\delta \dot{m}'')_i * [NO_i]$$

$$M_{IN} = M_{IN} + (\delta \dot{m}'')_i + \dot{R}_i$$

44. If this is not the last element in the array satisfying the criteria $1 \le i \le i_{MAX}$ increment i as i = i + 1 and go to step 30. If this is the last element, go to step 45.

45. Calculate $[NO]_{O-1}$ as:

$$[NO]_{O-1} = [NO]_{O-1} + [NO]_{O-2} / \delta X$$

46. Calculate rat_1 as:

$$rat_1 = [NO]_{O-1} / M_{IN}$$

47. Initialize $\Sigma_{NO/i}$ as:

$$\Sigma_{NO/i} = 0$$

48. Set i = 1.

Step 49 is performed only if $(\delta \dot{m}_i)_D = 0$ or if the chemical rate of production of NO in the element is zero.

49. Go to step 55.

50. Calculate $[NO_i']$ as:

$$[NO_i'] = rat_1$$

51. Using Subroutine RUNKUT, calculate the values of $[NO_i]$ and q_i at X_D.

Step 52 is performed only if $[NO_i] < 0$

52. Calculate $[NO_i]$ as:

$$[NO_i] = rat_1$$

53. Calculate $\Sigma_{NO/i}$ as:

$$\Sigma_{NO/i} = \Sigma_{NO/i} + [NO_i] * (\Delta m_i)_D$$

54. Recalculate X_U as:

$X_U = X_D - \delta X$

55. If this is not the last element in the array satisfying the criteria $1 \leq i \leq i_{MAX}$ increment i as i = i + 1 and go to step 49. If this is the last element, go to step 56.

56. Calculate $\overline{NO}$ as

$$\overline{NO} = \Sigma_{NO/i} / m_D^*$$

57. Set X_U equal to X_D.

58. If $II < N$, increment II as II = II + 1 and go to step 24 to continue the integration. If not, go to step 59.

59. Set i = 1.

60. Calculate D_ρ and $[NO]_{gm}$ as:

$$D_\rho = \rho_i * (\Delta m_i)_D$$

$$[NO]_{gm} = [NO_i] * (\Delta m_i)_D$$

61. Calculate $(\Sigma_1)_j$ and $(\Sigma_2)_j$ as:

$$(\Sigma_1)_j = (\Sigma_1)_j + D_\rho$$

$$(\Sigma_2)_j = (\Sigma_2)_j + [NO]_{gm}$$

62. If this is not the last element in the array satisfying the criteria $1 \leq i \leq i_{MAX}$ increment i as i = i + 1 and go to step 60. If this is the last element, go to step 63.

63. Calculate the mass average density, $\bar{\rho}_j$, and the mass average nitric oxide concentration $\overline{NO}_j$ for the jth iteration as:

$$\bar{\rho}_j = (\Sigma_1)_j / m_D^*$$
$$\overline{NO}_j = (\Sigma_2)_j / m_D^*$$

Step 64 is performed only if intermediate output is requested by the user.

64. Write X_D, J, $\bar{\rho}_j$ and $\overline{NO}_j$.

Steps 65-66 are performed only if J = 1.

65. Calculate $[NO]_{DUM}$ as:

$$[NO]_{DUM} = \overline{NO}$$

66. Go to step 69.

Steps 67-71 are performed only if 1 < J < 5.

67. Calculate $[\Delta NO]$ as:

$$[\Delta NO] = \frac{\overline{NO} - [NO]_{DUM}}{\overline{NO}}$$

Step 68 is performed only if $[\Delta NO] < 0.01$

68. Go to step 74.

69. Reset J and N as:

    J = J + 1

    N = 2N

70. Set $[NO]_{DUM} = \overline{NO}$.

71. Go to step 17.

Steps 72-73 are performed only if $5 \leq J \leq 6$.

72. Calculate $[\Delta NO]$ as:

$$[\Delta NO] = \left| \frac{\overline{NO} - [NO]_{DUM}}{\overline{NO}} \right|$$

73. Write $[\Delta NO]$, N, and X_D with the error message indicating that the Runge-Kutta iteration failed to converge to the specified limit.

Step 74 is performed only if II = N and this is the last major integration step in the intermediate zone.

74. Go to step 119.

75. Calculate $[\overline{NO}]$, $\bar{\rho}$, $\bar{T}$, $(\bar{C}_{(s)})_e$, $(\overline{CO})_e$ and $(\overline{CH_2})_e$ as:

$$[\overline{NO}] = \sum_{i=1}^{i_{MAX}} [NO_i] * (\Delta m_i)_D / M_D^*$$

$$\bar{\rho} = \sum_{i=1}^{i_{MAX}} \rho_i * (\Delta m_i)_D / M_D^*$$

$$\bar{T} = \sum_{i=1}^{i_{MAX}} T_i * (\Delta m_i)_D / M_D^*$$

$$(\bar{C}_{(s)})_e = \sum_{i=1}^{i_{MAX}} ((C_{(s)})_i)_e * (\Delta m_i)_D / M_D^*$$

$$(\overline{CO})_e = \sum_{i=1}^{i_{MAX}} (CO_i)_e * (\Delta m_i)_D / M_D^*$$

$$(\overline{CH_2})_e = \sum_{i=1}^{i_{MAX}} (CH_{2_i})_e * (\Delta m_i)_D / M_D^*$$

76. Calculate $\overline{MW}$ as:

$$\overline{MW} = \bar{\rho} * \bar{T} * 82.057 / P$$

77. Calculate $[\bar{C}_{(s)}]_e$, $[\overline{CO}]_e$, and $[\overline{CH_2}]_e$ as:

$$[\bar{C}_{(s)}]_e = (\bar{C}_{(s)})_e * 12 / \overline{MW}$$

$$[\overline{CO}]_e = (\overline{CO})_e * 28 / \overline{MW}$$

$$[\overline{CH_2}]_e = (\overline{CH_2})_e * 14 / \overline{MW}$$

78. Calculate $\{\overline{NO}\}$, $[\overline{NO}^*]$, and $\lceil\overline{NO}\rfloor$ as:

$$\{\overline{NO}\} = [\overline{NO}] * 10^6 * \overline{MW} / 30.0$$

$$[\overline{NO}^*] = [\overline{NO}] * \bar{\rho}$$

$$\lceil\overline{NO}\rfloor = [\overline{NO}] * M_D^* * 1000 / (\dot{M}_f)_{x_D}$$

79. Calculate $\{\bar{C}_{(s)}\}_e$, $\{\bar{CO}\}_e$; and $\{\bar{CH_2}\}_e$ as:

$$\{\bar{C}_{(s)}\}_e = [\bar{C}_{(s)}]_e * 10^6 * \bar{MW}/12$$

$$\{\bar{CO}\}_e = [\bar{CO}]_e * 10^6 * \bar{MW}/28$$

$$\{\bar{CH_2}\}_e = [\bar{CH_2}]_e * 10^6 * \bar{MW}/14$$

80. Calculate $[\bar{C}^*_{(s)}]_e$, $[\bar{CO}^*]_e$, and $[\bar{CH}^*_2]_e$ as:

$$[\bar{C}^*_{(s)}]_e = [\bar{C}_{(s)}]_e * \bar{\rho}$$

$$[\bar{CO}^*]_e = [\bar{CO}]_e * \bar{\rho}$$

$$[CH_2^*]_e = [\bar{CH_2}]_e * \bar{\rho}$$

81. Calculate $\lceil \bar{C}_{(s)} \rfloor_e$, $\lceil \bar{CO} \rfloor_e$ and $\lceil \bar{CH_2} \rfloor_e$ as:

$$\lceil \bar{C}_{(s)} \rfloor_e = [\bar{C}_{(s)}]_e * M_D^* * 1000 / (\dot{M}_F)_{x_D}$$

$$\lceil \bar{CO} \rfloor_e = [\bar{CO}]_e * M_D^* * 1000 / (\dot{M}_F)_{x_D}$$

$$\lceil \bar{CH_2} \rfloor_e = [\bar{CH_2}]_e * M_D^* * 1000 / (\dot{M}_F)_{x_D}$$

82. Calculate $[\Delta \bar{NO}]_{\Delta X}$ as:

$$[\Delta \bar{NO}]_{\Delta X} = \frac{\lceil \bar{NO} \rfloor - \lceil \bar{NO} \rfloor_{OP}}{\lceil \bar{NO} \rfloor}$$

83. Calculate n_{step} as:

$$n_{step} = (X_{END} - X_J)/\Delta X$$

Step 84 is performed only if $([\Delta \bar{NO}]_{\Delta X} * n_{step}) < 0.05$

84. Set the appropriate indicator to indicate that the nitric oxide reaction is frozen at this point in the combustor.

85. Calculate $\tilde{\Upsilon}_{inc}$ as:

$$\tilde{\Upsilon}_{inc} = \Delta X * \bar{\rho} * A|_{x_D} / \dot{m}_D^*$$

86. Calculate $\bar{\tilde{\Upsilon}}_{int}$ and $\tilde{\Upsilon}$ as:

$$\tilde{\Upsilon}_{int} = \tilde{\Upsilon}_{int} + \tilde{\Upsilon}_{inc}$$

$$\tilde{\Upsilon} = \tilde{\Upsilon} + \tilde{\Upsilon}_{inc}$$

87. Calculate V as:

$$V = \dot{m}_D^* / \bar{\rho} * A|_{x_D}$$

88. Calculate $\bar{\varphi}$ as:

$$\bar{\Phi} = \bar{F} / (K_S * (1 - \bar{F}))$$

89. Using Subroutine PRINTS, write the output for this axial station in the intermediate zone.

Step 90 is performed only if the nitric oxide reaction is frozen at this point in the combustor.

90. Write a message indicating frozen conditions exist in the combustor.

Step 91 is performed only if the appropriate indicator has been previously set to indicate that the nitric oxide reaction is frozen.

91. Go to step 124.

92. Set $[\bar{NO}]_{UP}$ as:

$$[\bar{NO}]_{UP} = [\bar{NO}]$$

93. Calculate $(\bar{\rho})_{rr}$ as:

$$(\bar{\rho})_{rr} = \bar{\rho}$$

Step 94 is performed only for the last major integration step in the intermediate zone.

94. Go to step 125.

95. Calculate X_{XXX} as:

$X_{XXX} = X_L - X_U$ if intermediate zone calculations end at X_L.

$X_{XXX} = X_{END} - X_U$ if intermediate zone calculations end at X_{END}.

Step 96 is performed only if $\Delta X < X_{XXX}$

96. Go to step 12.

97. Calculate ΔX as:

$$\Delta X = X_{XXX}$$

98. Set the appropriate indicator to indicate that this is the last major integration step in the intermediate zone.

99. Go to step 12.

100. Set the appropriate indicator to indicate a dilution zone type calculation is to be applied to the last element in the intermediate zone.

101. Using Subroutine ZMASS, calculate the over-all mass flow rate, the mean mixture ratio, and the airflow rate at X_D.

102. Using Subroutine CHECKK, calculate the mass flow rate out of an element due to mixing and the total mass flowing into it.

103. Reset the appropriate indicator to indicate intermediate zone calculations.

104. Calculate Q and $[NO]_{AN}$ as:

$$Q = \sum_{i=1}^{i_{MAX}} q_i * (\Delta m_i)_D / M^*_D$$

$$[NO]_{AN} = \sum_{i=1}^{i_{MAX}} [NO_i] * (\Delta m_i)_D / M^*_D$$

105. Using Subroutine MINT, calculate $(R_1)_{LST}$

106. Using Subroutine MINT, calculate $(R_6)_{LST}$

107. Using Subroutine MINT, calculate $(K_1)_{LST}$

108. Using Subroutine MINT, calculate $(K_2)_{LST}$

109. Using Subroutine MINT, calculate $(NO_2)_{LST}$

110. Using Subroutine MINT, calculate ρ_{LST}

111. Using Subroutine MINT, calculate T_{LST}

112. Calculate $[NO]_{IK}$ as:

$$[NO]_{IK} = (NO_2)_{LST} * 30.0 / \rho_{LST} * T_{LST} * 82.057 / P$$

113. Set the appropriate indicator to indicate that this is the last step of the intermediate zone calculations.

114. Using Subroutine RUNKUT, compute the values of $[\widetilde{NO}]_{AN}$ and Q at X_D.

115. Recalculate X_U as:

$$X_U = X_D - \delta X$$

116. Reset the appropriate indicator to signify intermediate zone calculations.

117. Calculate $\bar{\rho}_j$ and $\overline{NO}_j$ as:

$$\bar{\rho}_j = \rho_{LST}$$

$$\overline{NO}_j = [\widetilde{NO}]_{AN}$$

118. Go to step 65.

119. Compute $\bar{\bar{T}}$, $\bar{\rho}$ and $[\overline{NO}]$ as:

$$\bar{\bar{T}} = T_{LST}$$

$$\bar{\rho} = \rho_{LST}$$

$$[\overline{NO}] = [\widetilde{NO}]_{AN}$$

120. Using Subroutine MINT, compute $(\bar{C}_{(s)})_e$.

121. Using Subroutine MINT, compute $(\overline{CO})_e$.

122. Using Subroutine MINT, compute $(\overline{CH}_2)_e$.

123. Go to step 76.

124. Calculate $[\widetilde{NO}]_{AN}$ as:

$$[\widetilde{NO}]_{AN} = [\widetilde{NO}]$$

125. Return.

```
      SUBROUTINE ZINTER
      REAL NONO(50),MSTARU,MSTARD,NO,NOAVGS,NOP,NOSTAR
      DIMENSION AVRHO(10),AVNO(10),KON(10),Q(50),QQ(50),SUM1(10),SUM2(10
     1)
      COMMON/DATA1/AIR(50),RR(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(
     150),ZP(70),CUMDIS(70),VP,RHO(50),BCON6(50),ATT(50),PPP,FNOXP,R1(50
     2),R6(50),EK1(50),EK2(50),A2,A3,XL,CN,BETA,S,PHIP,EKS,XEND,A1
      COMMON/OUT1/AVECSG,AVECOG,AVCH2G,AVECSP,AVECOP,AVCH2P,AVECSD,AVECO
     1D,AVCH2D,AVECSF,AVECOF,AVCH2F
      COMMON/OUT2/AVENOG,AVENOD,AVENOP,AVENOF,AVENFU,RRO,ILAST
      COMMON/OUT3/INDIC,NO(50),AVET,TAUBAR,RHOBAR,PHIBAR,IMAX,XD,
     1FBARD,XU,LEN,TAUINT,TAUDIL,VELOC
      COMMON/OUT4/CONGNO(50),DELMD(50),AREAD,ASLOPE,DMFUO,SLOPE(50),TSLO
     1PE,NOP(50),EKKD,DMFT,UDM(50),ODM(50),      FB(50),DMFUD,AIRD,DMFFED
     2,RSUBX,SIG,SIGZER,AVEMW,DMDDA(50),DMDDM(50),DMDDP(50),DMDDPP(50),F
     3PRIME(50),NOEQXD,ANO,AQQ,SUEA(50),NOZERO(50),RDOT(50),E(50)
      COMMON/OUT5/MSTARD,MSTARU
      COMMON/OUT6/REAT,DILL
C****
C**** SET INITIAL INDICATORS,CALCULATE DELTAX,CHECK X
C****
      NPRINT=0
      ILAST=0
      LSGN = 1
      INDIC = 2
      IENDZ=0
      AVENFU=0.0
      EK=0.05
      XU = XD
      TAUINT = 0.0
      DO 100 I =1,50
      Q(I) = 1.0E-15
  100 CONTINUE
      DELTAX = 0.1*RSUBX
      IF(LEN.EQ.0) XI=XL-XU
      IF(LEN.EQ.1) XI = XEND-XU
      IF(DELTAX.LE.XI) GO TO 200
      DELTAX = XI
      IENDZ = 1
  200 CONTINUE
C****
C**** STORE INITIAL VALUES FOR BEGINNING OF EACH MAJOR STEP
C****
  250 CONTINUE
      DO 300 I = 1,50
      NONO(I) = NO(I)
      QQ(I) = Q(I)
      KON(I) = 0
  300 CONTINUE
      DO 350 K =1,6
      SUM1(K) = 0.0
      SUM2(K) = 0.0
  350 CONTINUE
      XXX = XD
      J = 1
      N=5
C****
C**** SET INITIAL VALUES EQUAL TO STORED VALUES EACH TIME N CHANGES
C****
  360 CONTINUE
```

```
      IF(J.EQ.1) GO TO 500
      XU = XXX
C****
C**** RESET UDM(I) FOR CALCULATION OF SLOPE
C****
      XD=XU
      CALL ZMASS(DELX)
      DO 400 I = 1,IMAX
      NO(I) = NONO(I)
      Q(I) = QQ(I)
  400 CONTINUE
  500 EN = N
      DELX = DELTAX/EN
      EMKO=CA/XL
      AVVNOG=AVENOG
C****
C**** START THE MAJOR STEPS DOWN THE COMBUSTOR
C****
      DO 3000 II =1,N
      OUTNO=0.0
      OUTNO2=0.0
      PINO=0.0
      XD = XU+DELX
      IF(II.EQ.N.AND.IENDZ.EQ.1) GO TO 8000
      CALL ZMASS(DELX)
      CALL CHECKK(DELX)
C****
C**** TEST EACH ELEMENT FOR CONVERGENCE
C****
C****
C**** IF NOZERO=1  BYPASS THE NO CALC
C****
      DO 2000 I=1,IMAX
      IIE=0
      IF(SLOPE(I).LT.0.0.AND.DDM(I).EQ.0.0) OUTNO2=OUTNO2+UDM(I)*NO(I)
      IF(DDM(I).EQ.0.0) GO TO 2000
      DMDDA(I) = UDM(I)*ASLOPE/HSTARU
  600 DMDDP(I)=SLOPE(I)+E(I)*UDM(I)   -RDOT(I)
      DMDDM(I)=DMDDP(I)-DMDDA(I)
      DMDDPP(I) = E(I)*UDM(I)
      IF(DMDDM(I).GT.0.0) GO TO 700
      E(I)=2.0*E(I)
C****
C**** CN,HENCE E(I).CANNOT EQUAL ZERO
C****
      IF(E(I).EQ.0.0) E(I)=0.02
      IIE=IIE+1
      IF(IIE.LT.40) GO TO 600
      WRITE(6,9999) IIE,E(I)
      LEN=1
      GO TO 9000
  700 CONTINUE
      OUTNO=OUTNO+DMDDPP(I)*NO(I)
      PINO=PINO+DMDDP(I)+RDOT(I)
 2000 CONTINUE
      OUTNO=OUTNO+OUTNO2/DELX
      AVVNO=OUTNO/PINO
      SUMNOI=0.0
      DO 4000 IJ=1,IMAX
      IF(DDM(IJ).EQ.0.0) GO TO 4000
```

```
      IF(NOZERO(IJ).EQ.1) GO TO 4000
      NOP(IJ)=AVVNO
      CALL RUNKUT(XU,DELX,NO(IJ),Q(IJ),LSGN,IJ)
      IF(NO(IJ).LT.0.0) NO(IJ)=AVVNO
      SUMNOI = SUMNOI+NO(IJ)*DELMD(IJ)
      XU=XU-DELX
 4000 CONTINUE
      AVVNOG=SUMNOI/MSTARD
      XU=XD
 3000 CONTINUE
      DO 3500 I =1,IMAX
      RHOMI = RHO(I)*DELMD(I)
      GNOMI = NO(I)*DELMD(I)
      SUM1(J) = SUM1(J)+RHOMI
      SUM2(J) = SUM2(J)+GNOMI
 3500 CONTINUE
      AVRHO(J) = SUM1(J)/MSTARD
      AVNO(J) = SUM2(J)/MSTARD
C****
C**** WRITE CONTROL
C****
      IF(NPRINT.EQ.0) GO TO 3550
      WRITE(6,3600) XD,J,AVRHO(J),AVNO(J)
 3600 FORMAT(9H X(CM) = ,E12.5,4HJ = ,I2,18HAVE. RHO(GM/CC) = ,E12.5,17H
     1AVE. NO(GM/GM) = ,E12.5)
 3550 CONTINUE
C****
C**** LOGIC CONTROL ON J
C****
      GO TO (4100,4300,4300,4300,4600,4600),J
 4100 DUMMY=AVVNOG
      GO TO 4500
 4300 DIFNO=ABS((AVVNOG-DUMMY)/AVVNOG)
      IF(DIFNO.LT.0.01 ) GO TO 5000
 4500 J= J+1
      N = 2*N
      DUMMY=AVVNOG
      GO TO 360
 4600 DDFNO=ABS((AVVNOG-DUMMY)/AVVNOG)
      WRITE(6,4700) DDFNO,N,XD
 4700 FORMAT(///,69H RUNGE-KUTTA ITERATION FAILED TO CONVERGE TO SPECIF
     1ED LIMIT.DIFNO = ,E12.5,5H N = ,I4,5H X = ,E12.5,5H CMS.///)
 4800 CONTINUE
 5000 CONTINUE
      IF(II.EQ.N.AND.IENDZ.EQ.1) GO TO 8500
C****
C**** WRITE THE APPROPRIATE OUTPUT FOR THIS AXIAL STATION
C****
      AVENOG = 0.0
      RHOBAR = 0.0
      AVET = 0.0
      CSAV = 0.0
      COAV = 0.0
      CH2AV = 0.0
      DO 6000 I =1,IMAX
      AVENOG = AVENOG+NO(I)*DELMD(I)
      RHOBAR = RHOBAR+RHO(I)*DELMD(I)
      AVET = AVET+ATT(I)*DELMD(I)
      CSAV = CSAV+BCON1(I)*DELMD(I)
      COAV = COAV+BCON2(I)*DELMD(I)
```

```
      CH2AV = CH2AV+CH2(I)*DELMD(I)
 6000 CONTINUE
      AVENOG = AVENOG/MSTARD
      RHOBAR = RHOBAR/MSTARD
      AVET = AVET/MSTARD
      CSAV = CSAV/MSTARD
      COAV = COAV/MSTARD
      CH2AV = CH2AV/MSTARD
 6500 AVEMW = RHOBAR*AVET*82.057/PPP
      AVECSG = CSAV*12.0/AVEMW
      AVECOG = COAV*28.0/AVEMW
      AVCH2G = CH2AV*14.0/AVEMW
      AVENOP=AVENOG*1.0E+06*AVEMW/30.0
      AVENOD = AVENOG*RHOBAR
      AVENOF = AVENOG*MSTARD*1000./DMFT
      AVECSP=AVECSG*1.0E+06*AVEMW/12.0
      AVECOP=AVECOG*1.0E+06*AVEMW/28.0
      AVCH2P=AVCH2G*1.0E-06*AVEMW/14.0
      AVECSD = AVECSG*RHOBAR
      AVECOD = AVECOG*RHOBAR
      AVCH2D = AVCH2G*RHOBAR
      AVECSF = AVECSG*MSTARD*1000./DMFT
      AVECOF = AVECOG*MSTARD*1000./DMFT
      AVCH2F = AVCH2G*MSTARD*1000./DMFT
      FURAT=(AVENOF-AVENFU)/AVENOF
      STEPS=(XEND-XU)/DELTAX
      IF(FURAT*STEPS.LT.0.05) ILAST=1
C****
C**** CALCULATE RESIDENCE TIME,ETC.
C****
      TAU = DELTAX*RHOBAR*AREAD/MSTARD
      TAUINT = TAUINT+TAU
      TAUBAR = TAUBAR+TAU
      VELOC = MSTARD/(RHOBAR*AREAD)
      PHIBAR = FBARD/(EKS*(1.0-FBARD))
      CALL PRINTS
      IF(ILAST.EQ.1) WRITE(6,9500)
 9500 FORMAT(/////,10X,42HNITRIC OXIDE REACTION FROZEN AT THIS POINT,///
     1)
      IF(ILAST.EQ.1) GO TO 8600
C****
C**** CONTROL OVERALL STEPS
C****
      AVENFU=AVENOF
      RRO=RHOBAR
      IF(IENDZ.EQ.1) GO TO 9000
      IF(LEN.EQ.0) XXXX = XL-XU
      IF(LEN.EQ.1) XXXX = XEND-XU
      IF(DELTAX.LT.XXXX) GO TO 250
      DELTAX = XXXX
      IENDZ = 1
      GO TO 250
C****
C**** COMPUTATION FOR LAST ELEMENT
C****
 9000 INDIC = 3
      CALL ZMASS(DELX)
      CALL CHECKK(DELX)
      INDIC = 2
      AQQ = 0.0
```

```
      ANO = 0.0
      DO 8100 I =1,IMAX
      AQQ = AQQ+Q(I)*DELMD(I)
      ANO = ANO+NO(I)*DELMD(I)
 8100 FFF = FBARD
      AQQ = AQQ/MSTARD
      ANO = ANO/MSTARD
      CALL MINT(1,FFF,35,FF,R1,R1LAST)
      CALL MINT(1,FFF,35,FF,R6,R6LAST)
      CALL MINT(1,FFF,35,FF,EK1,EK1LST)
      CALL MINT(1,FFF,35,FF,EK2,EK2LST)
      CALL MINT(1,FFF,35,FF,BCON6,YNOLST)
      CALL MINT(1,FFF,35,FF,RHO,RHOLST)
      CALL MINT(1,FFF,35,FF,ATT,TTLAST)
      CNOLST = YNOLST*30.0/(RHOLST* TTLAST*82.057/PPP)
      STORE1 = R1(1)
      STORE2 = R6(1)
      STORE3 = EK1(1)
      STORE4 = EK2(1)
      STORE5 = CONGNO(1)
      STORE6 = ATT(1)
      STORE7 = RHO(1)
      R1(1) = R1LAST
      R6(1) = R6LAST
      EK1(1) = EK1LST
      EK2(1) = EK2LST
      RHO(1) = RHOLST
      ATT(1) = TTLAST
      CONGNO(1) = CNOLST
      LSGN = 2
      CALL RUNKUT(XU,DELX,ANO,AQQ,LSGN,1)
      XU = XU-DELX
      R1(1) = STORE1
      R6(1) = STORE2
      EK1(1) = STORE3
      EK2(1) = STORE4
      CONGNO(1) = STORE5
      ATT(1) = STORE6
      RHO(1) = STORE7
      AVRHO(J) = RHOLST
      AVNO(J) = ANO
      LSGN = 1
      GO TO 3550
C****
C**** COMPUTE APPROPRIATE AVERAGES
C****
 6500 AVET = TTLAST
      RHOBAR = RHOLST
      AVENOG = ANO
      CALL MINT(1,FFF,35,FF,BCON1,CSAV)
      CALL MINT(1,FFF,35,FF,BCON2,COAV)
      CALL MINT(1,FFF,35,FF,CH2,CH2AV)
      GO TO 6550
 9999 FORMAT(10X,I6,8E12.5)
 8600 ANO=AVENOG
 9000 RETURN
      END
```

APPENDIX VI - SUBROUTINE DILUTE

The function of Subroutine DILUTE is to calculate the concentration of nitric oxide at specified axial stations, and at the exit of the dilution zone of a gas turbine combustor.

Subroutine DILUTE is called by the main routine (GASNOX); it, in turn, calls Subroutines ZMASS, MINT, RUNKUT, and PRINTS. The subroutine does not require external input but does provide external output. Internal input and output are transmitted through COMMON. The internal input consists of:

AIRD	ANO	AQQ	ATT	BCON1
BCON2	BCON6	CH2	EKS	EK1
EK2	FF	ILAST	PPP	RHO
RSUBX	R1	R6	S	XEND
XD				

The internal output consists of:

ANO	AVCH2D	AVCH2F	AVCH2G	AVCH2P
AVECOD	AVECOF	AVECOG	AVECOP	AVECSD
AVECSF	AVECSG	AVECSP	AVEMW	AVENFU
AVENOD	AVENOF	AVENOG	AVENOP	AVET
INDIC	NOEQXD	PHIBAR	RRO	TAUBAR
TAUDIL	VELOC	XD	XU	

The external output consists of:

DDIFNO	DILL	DNO	J	N
REAT	RHOBAR	XD		

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols used in Subroutine DILUTE which are not included in COMMON.

Fortran Symbol	Symbol	Description	Units
AIRXX	$M_A]_X$	Combustor airflow at axial station X_D	gm/sec
DDIFNO	$[\Delta NO]$	Difference in NO concentrations for successive iterations at the end of each major step in the combustor	

Fortran Symbol	Symbol	Description	Units
DELTAX	ΔX	Integration step size (major) in the dilution zone	cm
DELX	δX	Increment of the combustor length across which the solution is generated	cm
DNO	$[\overline{NO}]_{DN}$	Average NO at given axial station (downstream) in the combustor	
DUMMY	$[NO]_{DUM}$	Dummy variable	
EK1LST	$(K_1)_{LST}$	Ratio of forward reaction rate constants at a given axial station in the dilution zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)	
EK2LST	$(K_2)_{LST}$	Ratio of forward reaction rate constants at a given axial position in the dilution zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)	
EN	N	Proportionality constant between ΔX and δX	
FURAT	$[\Delta NO]_{\Delta X}$	Measure of change in NO concentration for successive steps in the combustor	
IENDD		Indicator IENDD = 0 for all except the last major integration step in the dilution zone IENDD = 1 for the last major integration step in the dilution zone	
II	II	Integration increment index	
J	J	Number of iterations for each major axial step in the combustor	
LSGN		Indicator LSGN = 1 if intermediate zone and not the last step in the zone LSGN = 2 if intermediate zone and the last step in the zone LSGN = 3 if dilution zone	
N	N	Proportionality constant between ΔX and $\hat{\delta} X$	
NONO	$[\overline{NO}]_{NO}$	Dummy variable	

Fortran Symbol	Symbol	Description	Units
NPRINT		Indicator NPRINT = 0 if intermediate output is not requested by the user NPRINT = 1 if intermediate output is requested by the user	
Q	q	Measure of the round-off error in the Runge-Kutta integration routine at a given axial station in the combustor	
QQ	qq	Measure of the round-off error in the Runge-Kutta integration routine at a given axial station	
R1LST	$(R_1)_{LST}$	Forward reaction rate for the first kinetic reaction at a given axial position in the dilution zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)	gm-mole/cm^3-sec
R6LST	$(R_6)_{LST}$	Forward reaction rate for the sixth kinetic reaction at a given axial position in the dilution zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)	gm-mole/cm^3-sec
STEPS	n_{step}	Number of remaining integration steps before combustor exit	
STORE1		Dummy variable	gm-mole/cm^3-sec
STORE2		Dummy variable	gm-mole/cm^3-sec
STORE3		Dummy variable	
STORE4		Dummy variable	
TAU	$\bar{\tau}_{inc}$	Incremental residence time	sec
XDZ	X_{DZ}	Distance between upstream end of integration interval to combustor exit	cm
XXX	X_{XX}	Axial position in the combustor	cm
XXXX	X_{XXX}	Distance between upstream end of integration interval and combustor exit	cm
YCH2XD	$(CH_2)_{ex_D}$	Equilibrium mole fraction of unburned hydrocarbon (exclusive of $C_{(s)}$ and CO) at a given axial station in the dilution zone at the mean mixture ratio	

Fortran Symbol	Symbol	Description	Units
YCOXD	$(CO)_{eX_D}$	Equilibrium mole fraction of CO at a given axial station in the dilution zone at the mean mixture ratio	
YCSXD	$(C_{(s)})_{eX_D}$	Equilibrium mole fraction of $C_{(s)}$ at a given axial station in the dilution zone at the mean mixture ratio	
YNOXD	$(NO)_{eX_D}$	Equilibrium mole fraction of NO at a given axial station in the dilution zone at the mean mixture ratio	

Analysis Procedure

The step-by-step procedure of Subroutine DILUTE is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Initialize indicators.
2. Set $[\overline{NO}]_{DN} = [\overline{NO}]_{AN}$

Step 3 is performed only if the nitric oxide reaction is frozen at the point in the combustor.

3. Go to step 16
4. Calculate X_U, $\tilde{\Upsilon}_{DIL}$, and q as:

$X_U = X_D$

$\tilde{\Upsilon}_{DIL} = 0$

$q = Q$

5. Calculate ΔX and X_{DZ} as:

$$\Delta X = 0.1 * R_{X_D}$$

$$X_{DZ} = X_{END} - X_U$$

Step 6 is performed if $\Delta X \leq X_{DZ}$

6. Go to step 8.
7. Set the indicator to indicate that this is the last step in the combustor and calculate ΔX as:

$$\Delta X = X_{DZ}$$

8. Initialize dummy variables $\mathfrak{M}_A\big|_{DX}$ and $[\overline{NO}]_{NO}$ as:

$$\mathfrak{M}_A\big|_{\Delta X} = \mathfrak{M}_A\big|_{X_D}$$

$$[\overline{NO}]_{NO} = [\overline{NO}]_{DN}$$

9. Initialize qq and X_{XX} as:

$qq = q$

$X_{XX} = X_D$

10. Initialize J and N as:

$J = 1$

$N = 20$

11. Initialize II as:

$II = 1$

Step 12 is performed only if J = 1.

12. Go to step 14.

13. Calculate $\dot{M}_A|_{X_D}$, X_U, q, and $[NO]_{DN}$ as:

$$\dot{M}_A|_{X_D} = \dot{M}_A|_{XX}$$
$$X_U = X_{XX}$$
$$q = qq$$
$$[NO]_{DN} = [NO]_{NO}$$

14. Calculate δX as:

$\delta X = \Delta X/N$

15. Go to step 19.

16. Set N, II, and J as:

$N = 10$

$II = N$

$J = 6$

17. Calculate δX, ΔX and X_U as:

$$\delta X = X_{END} - X_U$$
$$\Delta X = \delta X$$
$$X_U = X_D$$

18. Calculate $[NO]_{AN}$ as:

$$[NO]_{AN} = [NO]_{DN}$$

19. Calculate X_D as:

$X_D = X_U + \delta X$

20. Using Subroutine ZMASS, calculate the over-all mass flow rate, mean mixture ratio, and airflow rate at X_D

21. Using Subroutine MINT, calculate $(R_1)_{LST}$

22. Using Subroutine MINT, calculate $(R_G)_{LST}$

23. Using Subroutine MINT, calculate $(K_1)_{LST}$

24. Using Subroutine MINT, calculate $(K_2)_{LST}$

25. Using Subroutine MINT, calculate $(NO)_{e x_D}$
26. Using Subroutine MINT, calculate $\bar{\rho}$
27. Using Subroutine MINT, calculate $\bar{T}$
28. Using Subroutine MINT, calculate $(C_{(s)})_{e x_D}$
29. Using Subroutine MINT, calculate $(CO)_{e x_D}$
30. Using Subroutine MINT, calculate $(CH_2)_{e x_D}$

Steps 31 and 32 are performed only if the nitric oxide reaction is frozen at this point in the combustor.

31. Calculate $[\overline{NO}]_{DN}$ as:

$$[\overline{NO}]_{DN} = [\overline{NO}]_{AN} * \left[M_D^* / M_P^*\right]$$

32. Go to step 38.
33. Calculate $[\overline{NO}_e]_{X_D}$ as:

$$[\overline{NO}_e]_{X_D} = (NO)_{e x_D} *$$

34. Using Subroutine RUNKUT, calculate the value of $[\overline{NO}]_{DN}$ and q

Steps 35 and 36 are performed only if II<N

35. Calculate II = II + 1
36. Return to step 20.

Step 37 is performed only if intermediate output is requested by the user.

37. Write X_D, J, $\bar{\rho}$, $[\overline{NO}]_{DN}$, $(\dot{r})_{react}$, $(\dot{r})_{DIL}$, $[\Delta NO]$, and N.

Steps 38 and 39 are performed only if J = 1

38. Calculate $[NO]_{DUM}$

$$[NO]_{DUM} = [\overline{NO}]_{DN}$$

39. Go to step 43.

Steps 40-42 are performed only if $1 < J < 5$.

40. Calculate $[\Delta NO]$ as:

$$[\Delta NO] = \left| \frac{([\overline{NO}]_{DN} - [NO]_{DUM})}{[\overline{NO}]_{DN}} \right|$$

Step 41 is performed only if $[\Delta NO] < 0.005$.

41. Go to step 48.
42. Reset $[NO]_{DUM}$ as:

$$[NO]_{DUM} = [\overline{NO}]_{DN}$$

43 Calculate J and N as

$J = J + 1$

$N = 2N$

44. Go to step 11.

Steps 45 and 46 are performed only if J = 5.

45. Write the error message stating that the Runge-Kutta iteration failed to converge. Write also the value of $[\Delta NO]$, N, and X_D:

46. Go to step 48.

Step 47 is performed only if J = 6.

47. Set the appropriate indicator to indicate that this is the last major step in the combustor.

48. Calculate $[\overline{NO}]$ as

$$[\overline{NO}] = [\overline{NO}]_{DN}$$

49. Calculate $\overline{MW}$ as

$$\overline{MW} = \bar{\rho} * \bar{T} * 82.057/P$$

50. Calculate $[\bar{C}_{(s)}]_e$, $[\overline{CO}]_e$, and $[\overline{CH_2}]_e$ as:

$$[\bar{C}_{(s)}]_e = (\bar{C}_{(s)})_{e x_D} * 12/\overline{MW}$$

$$[\overline{CO}]_e = (\overline{CO})_{e x_D} * 28/\overline{MW}$$

$$[\overline{CH_2}]_e = (\overline{CH_2})_{e x_D} * 14/\overline{MW}$$

51. Calculate $\{\overline{NO}\}$, $[\overline{NO}^*]$, and $[\overline{NO}]$ as:

$$\{\overline{NO}\} = [\overline{NO}] * 10^6 * \overline{MW}/30.0$$

$$[\overline{NO}^*] = [\overline{NO}] * \bar{\rho}$$

$$[\overline{NO}] = [\overline{NO}] * \dot{M}_D^* * 1000/(\dot{M}_f)_{x_D}$$

52. Calculate $\{\bar{C}_{(s)}\}_e$, $\{\overline{CO}\}_e$, and $\{\overline{CH_2}\}_e$ as:

$$\{\bar{C}_{(s)}\}_e = [\bar{C}_{(s)}]_e * 10^6 * \overline{MW}/12$$

$$\{\overline{CO}\}_e = [\overline{CO}]_e * 10^6 * \overline{MW}/28$$

$$\{\overline{CH_2}\}_e = [\overline{CH_2}]_e * 10^6 * \overline{MW}/14$$

53. Calculate $[\bar{C}_{(s)}^{*}]_e$, $[\bar{CO}^{*}]_e$, and $[\bar{CH}_2^{*}]_e$ as:

$$[\bar{C}_{(s)}^{*}]_e = [\bar{C}_{(s)}]_e * \bar{\rho}$$
$$[\bar{CO}^{*}]_e = [\bar{CO}]_e * \bar{\rho}$$
$$[\bar{CH}_2^{*}]_e = [\bar{CH}_2]_e * \bar{\rho}$$

54. Calculate $[\bar{C}_{(s)}]_e$, $[\bar{CO}]_e$, and $[\bar{CH}_2]_e$ as:

$$[\bar{C}_{(s)}]_e = [\bar{C}_{(s)}]_e * \dot{M}_D^* * 1000 / (\dot{M}_F)_{X_D}$$
$$[\bar{CO}]_e = [\bar{CO}]_e * \dot{M}_D^* * 1000 / (\dot{M}_F)_{X_D}$$
$$[\bar{CH}_2]_e = [\bar{CH}_2]_e * \dot{M}_D^* * 1000 / (\dot{M}_F)_{X_D}$$

Steps 55 and 56 are performed only if the nitric oxide reaction is frozen at this point in the combustor.

55. Calculate $\dot{M}_D^*$ as:

$$\dot{M}_D^* = \frac{1}{2}(\dot{M}_D^* + \dot{M}_U^*)$$

56. Calculate $\bar{\rho}$ as:

$$\bar{\rho} = \frac{1}{2}(\bar{\rho} + (\bar{\rho})_{rr})$$

57. Calculate $\bar{\tau}_{inc}$ as:

$$\bar{\tau}_{inc} = \Delta X * \bar{\rho} * A|_{X_D} / \dot{M}_D^*$$

58. Calculate $\bar{\tau}_{DIL}$ and $\bar{\tau}$ as:

$$\bar{\tau}_{DIL} = \bar{\tau}_{DIL} + \bar{\tau}_{inc}$$
$$\bar{\tau} = \bar{\tau} + \bar{\tau}_{inc}$$

59. Calculate V as:

$$V = \dot{M}_D^* / \bar{\rho} * A|_{X_D}$$

60. Calculate $\bar{\phi}$ as:

$$\bar{\phi} = \bar{F} / (k_s(1 - \bar{F}))$$

61. Calculate $[\Delta\overline{NO}]_{\Delta X}$ as:

$$[\Delta\overline{NO}]_{\Delta X} = \frac{[\overline{NO}] - [\overline{NO}]_{UP}}{[\overline{NO}]}$$

62. Calculate n_{step} as:

$$n_{step} = (X_{END} - X_U)/\Delta X$$

Step 63 is performed only if $\left([\Delta\overline{NO}]_{\Delta X} * n_{step}\right) < 0.05$

63. Set the appropriate indicator to indicate that the nitric oxide reaction is frozen at this point in the combustor.

64. Using Subroutine PRINTS, write the output for this axial station in the dilution zone.

65. Reset $[\overline{NO}]_{UP}$ as:

$$[\overline{NO}]_{UP} = [\overline{NO}]$$

66. Reset $(\bar{\rho})_{rr}$ as:

$$(\bar{\rho})_{rr} = \bar{\rho}$$

Step 67 is performed only if the appropriate indicator indicates that this is the last step in the dilution zone.

67. Go to step 75.

Step 68 is performed only if the nitric oxide reaction is frozen at this point in the combustor.

68. Write a message indicating frozen conditions exist in the combustor.

Step 69 is performed only if the appropriate indicator has been previously set to indicate that the nitric oxide reaction is frozen.

69. Go to step 16.

70. Calculate X_{XXX} as:

$X_{XXX} = X_{END} - X_D$.

Step 71 is performed only if $\Delta X < X_{XXX}$

71. Go to step 8.

72. Calculate ΔX as:

    $\Delta X = X_{XXX}$

73. Set the appropriate indicator to indicate that this is the last step in the dilution zon'.

74. Go to step 8.

75. Return.

```
      SUBROUTINE DILUTE
      REAL MSTARD,NO,NOEQXD,NONO,MSTARU
      COMMON/DATA1/AIR(50),RR(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(
     150),ZP(70),CUMDIS(70),VP,RHO(50),BCON6(50),ATT(50),PPP,FNOXP,R1(50
     2),R6(50),EK1(50),EK2(50),A2,A3,XL,CN,BETA,S,PHIP,EKS,XEND,A1
      COMMON/OUT1/AVECSG,AVECOG,AVCH2G,AVECSP,AVECOP,AVCH2P,AVECSD,AVECO
     1D,AVCH2D,AVECSF,AVECOF,AVCH2F
      COMMON/OUT2/AVENOG,AVENOD,AVENOP,AVENOF,AVENFU,RRO,ILAST
      COMMON/OUT3/INDIC,NO(50),AVET,TAUBAR,RHOBAR,PHIBAR,IMAX,XD,
     1FBARD,XU,LEN,TAUINT,TAUDIL,VELOC
      COMMON/OUT4/CONGNO(50),DELMO(50),AREAD,ASLOPE,DMFUO,SLOPE(50),TSLO
     1PE,NOP(50),EKKD,DMFT,UDM(50),DDM(50),      FB(50),DMFUD,AIRD,DMFFED
     2,RSUBX,SIG,SIGZER,AVEMW,DMDDA(50),DMDDM(50),DMDDP(50),DMDDPP(50),F
     3PRIME(50),NOEQXD,ANO,AQQ,DIFNO(50),NOZERO(50),ROOT(50),E(50)
      COMMON/OUT5/MSTARD,MSTARU
      COMMON/OUT6/REAT,DILL
C****
C**** SET INITIAL INDICATORS, CALCULATE DELTAX, CHECK X
C****
      NPRINT=0
      LSGN=3
      INDIC=3
      IENDD=0
      IF(S.EQ.0.0) ILAST=0
      DNO = ANO
      IF(ILAST.EQ.1) GO TO 2000
      XU=XD
      TAUDIL=0.0
      Q=AQQ
      DELTAX=0.1*RSUBX
      XDZ = XEND-XU
      IF(DELTAX.LE.XDZ) GO TO 200
      DELTAX = XDZ
      IENDD=1
  200 CONTINUE
C****
C**** STORE INITIAL VALUES FOR BEGINNING OF EACH MAJOR STEP
C****
  250 CONTINUE
      AIRXX = AIRD
      NONO = DNO
      QQ=Q
      XXX = XD
      J=1
      N=20
      DDIFNO = 0.0
C****
C****   SET INITIAL VALUES EQUAL TO STORED VALUES EACH TIME N CHANGES
C****
  300 II=1
      IF(J.EQ.1) GO TO 400
      AIRD = AIRXX
      XU=XXX
      Q=QQ
      DNO = NONO
  400 EN=N
      DELX=DELTAX/EN
C****
C**** START THE MAJOR STEPS DOWN THE COMBUSTOR
C****
```

```
      GO TO 2500
 2000 N=10
      II=N
      J=6
      DELX=XEND-XD
      DELTAX=DELX
      XU=XD
      ANO=DNO
 2500 DO 3000 II=1,N
      XD=XU+DELX
      CALL ZMASS(DELX)
C****
C**** CALCULATE NO AT XD
C****
      CALL MINT(1,FBARD,35,FF,R1,R1LST)
      CALL MINT(1,FBARD,35,FF,R6,R6LST)
      CALL MINT(1,FBARD,35,FF,EK1,EK1LST)
      CALL MINT(1,FBARD,35,FF,EK2,EK2LST)
      CALL MINT(1,FBARD,35,FF,BCON6,YNOXD)
      CALL MINT(1,FBARD,35,FF,RHO,RHOBAR)
      CALL MINT(1,FBARD,35,FF,ATT,AVET)
      CALL MINT(1,FBARD,35,FF,BCON1,YCSXD)
      CALL MINT(1,FBARD,35,FF,BCON2,YCOXD)
      CALL MINT(1,FBARD,35,FF,CH2,YCH2XD)
      IF(ILAST.EQ.1) DNO=ANO*MSTARU/MSTARD
      IF(ILAST.EQ.1) GO TO 4000
      STORE1 = R1(1)
      STORE2 = R6(1)
      STORE3 = EK1(1)
      STORE4 = EK2(1)
      R1(1) = R1LST
      R6(1) = R6LST
      EK1(1) = EK1LST
      EK2(1) = EK2LST
      NOEQXD=YNOXD*30.0/(RHOBAR*AVET*82.057/PPP)
      CALL RUNKUT(XU,DELX,DNO,Q,LSGN,1)
      R1(1) = STORE1
      R6(1) = STORE2
      EK1(1) = STORE3
      EK2(1) = STORE4
 3000 CONTINUE
C****
C**** WRITE CONTROL
C****
      IF(NPRINT.EQ.0) GO TO 4000
      WRITE(6,3500) XD,J,RHOBAR,DNO,REAT,DIL
      WRITE(6,9997) DDIFNO,N
 3500 FORMAT(9H X(CM) = ,E12.5,4HJ = ,I6,18HAVE. RHO(GM/CC) = ,E12.5,17H
     1AVE. NO(GM/CM) = ,E12.5,5X,2E12.5)
C****
C**** LOGIC CONTROL ON J
C****
 4000 CONTINUE
      GO TO (4100,4300,4300,4300,4600,4800), J
 4100 DUMMY = DNO
      GO TO 4500
 4300 DDIFNO = ABS((DNO-DUMMY)/DNO)
      IF(DDIFNO.LT.0.005) GO TO 5000
      DUMMY = DNO
 4500 J=J+1
```

```
      N=2*N
      GO TO 300
 4600 WRITE(6,4700) DDIFNO,N,XD
 4700 FORMAT(///,59H RUNGE-KUTTA ITERATION FAILED TO CONVERGE TO SPECIFI
     1ED LIMIT.DIFNO = ,E12.5,5H N = ,I4,5H X = ,E12.5,5H CMS.///)
      GO TO 5000
 4800 IENDD = 1
 5000 CONTINUE
C****
C**** WRITE THE APPROPRIATE OUTPUT FOR THIS AXIAL STATION
C****
      AVENOG = DNO
      AVEMW=RHOBAR*AVET*82.057/PPP
      AVECSG=YCSXD*12.0/AVEMW
      AVECOG=YCOXD*28.0/AVEMW
      AVCH2G=YCH2XD*14.0/AVEMW
      AVENOP=AVENOG*1.0E+06*AVEMW/30.0
      AVENOD=AVENOG*RHOBAR
      AVENOF=AVENOG*MSTARD*1000.0/DMFT
      AVECSP=AVECSG*1.0E+06*AVEMW/12.0
      AVECOP=AVECOG*1.0E+06*AVEMW/28.0
      AVCH2P=AVCH2G*1.0E+06*AVEMW/14.0
      AVECSD=AVECSG*RHOBAR
      AVECOD=AVECOG*RHOBAR
      AVCH2D=AVCH2G*RHOBAR
      AVECSF=AVECSG*MSTARD*1000.0/DMFT
      AVECOF=AVECOG*MSTARD*1000.0/DMFT
      AVCH2F=AVCH2G*MSTARD*1000.0/DMFT
C****
C**** CALCULATE RESIDENCE TIMES, ETC
C****
      IF(ILAST.EQ.1) MSTARD = 0.5*(MSTARU+MSTARD)
      IF(ILAST.EQ.1) RHOBAR=0.5*(RHOBAR+RRO)
      TAU = DELTAX*RHOBAR*AREAD/MSTARD
      TAUDIL=TAUDIL+TAU
      TAUBAR=TAUBAR+TAU
      VELOC=MSTARD/(RHOBAR*AREAD)
      PHIBAR=FBARD/(EKS*(1.0-FBARD))
      FURAT=(AVENOF-AVENFU)/AVENOF
      STEPS=(XEND-XU)/DELTAX
      IF(FURAT*STEPS.LT.0.05) ILAST = 1
      CALL PRINTS
C****
C**** CONTROL OVERALL STEPS
C****
      AVENFU=AVENOF
      RRO=RHOBAR
      IF(IENDD.EQ.1) GO TO 9000
      IF(ILAST.EQ.1) WRITE(6,9500)
 9500 FORMAT(/////,10X,42HNITRIC OXIDE REACTION FROZEN AT THIS POINT,///
     1)
      IF(ILAST.EQ.1) GO TO 2000
      XXXX=XEND-XU
      IF(DELTAX.LT.XXXX) GO TO 250
      DELTAX=XXXX
      IENDD=1
      GO TO 250
 9000 RETURN
 9997 FORMAT(20X,E10.3,I5)
      END
```

APPENDIX VII - SUBROUTINE PRCALC

The function of Subroutine PRCALC is to calculate the average nitric oxide level at the exit of the primary zone for each mixture ratio element.

Subroutine PRCALC is called by Subroutine PRIMRY; it, in turn, calls Subroutine MINY. Subroutine PRCALC does not require external input and does not provide external output except for an error message and diagnostic data table. External output is written directly onto the output-tape unit. Internal input and output are transmitted through COMMON and as arguments of the subroutine. The internal input consists of:

ATT	BCON1	BCON2	BCON6	CH2
CONGNO	DELMD	EK1	EK2	FBARD
FF	FNOXG	IMAX	NOZERO	PPP
RHO	R1	R6	S	

The internal output consists of:

AQQ	AVET	NO	NOEQXD	RHOBAR
TAUBAR				

The external output consists of:

ALPHA2	DUMMY		LIMIT	SUMTNO

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols in Subroutine PRCALC which are not included in COMMON.

Fortran Symbol	Symbol	Description	Units
AAA(I)	α_2	Ratio of NO concentration to NO concentration at equilibrium for a mixture element i at the end of the integration interval	
ALPHAD(I)	$(\alpha_D)_i$	Ratio of NO concentration to NO concentration at equilibrium for a mixture element i at the end of the integration interval	

Fortran Symbol	Symbol	Description	Units
ALPHAT(I)	$(\alpha_T)_i$	Ratio of NO concentration to NO concentration at equilibrium for a mixture element i at the mean primary zone residence time	
ALPHAU(I)	$(\alpha_U)_i$	Ratio of NO concentration to NO concentration at equilibrium for a mixture element i at the start of the integration interval	
ALPHA1	α_1	Ratio of NO concentration to NO concentration at equilibrium for a mixture element i at the start of the integration interval	
ALPHA2	α_2	Ratio of NO concentration to NO concentration at equilibrium for a mixture element i at the end of the integration interval	
ALPHD	$(\alpha_D)_i$	Ratio of NO concentration to NO concentration of equilibrium for a mixture element i at the end of integration interval	
ALPHU	$(\alpha_U)_i$	Ratio of NO concentration to NO concentration at equilibrium for a mixture element i at the start of the integration interval	
DALP	$(\Delta\alpha)_i$	Integration interval	
DALPHA	$(\Delta\alpha)_i$	Integration interval	
DUMMY(I)		Dummy variable	
EK1LST	$(K_1)_{LST}$	Ratio of forward reaction rate constants at mean primary zone mixture ratio (See Volume 2, Section 2 or Ref 3)	
EK2LST	$(K_2)_{LST}$	Ratio of forward reaction rate constants at mean primary zone mixture ratio (See Volume 2, Section 2 or Ref 3)	
EN	r	Integration step size control	
ERR	t_{err}	Convergence limit	
FNOXG	$[NO_G]$	NO formed in the flame front (mass fraction)	
FT	f_t	Fractional mass in an element that has a residence time dt about τ	

Fortran Symbol	Symbol	Description	Units
FTD	$(\xi_t)_D$	Accumulated mass fraction leaving element before t_D	
FTU	$(\xi_t)_U$	Accumulated mass fraction leaving element before t_U	
INDEX		Indicator: INDEX = 0 at start of iteration; INDEX = 1 if convergence criteria not satisfied	
J		Counter: J < 6 if convergence occurs on ε_{t-NO}; J = 6 if convergence limit is not satisfied on ε_{t-NO}	
JJ		Counter: JJ ≤ 20 if convergence test on $(\xi_t)_{rem}$ applied; JJ > 20 if convergence test on $(\xi_t)_{rem}$ not applied	
K		Indicator: K = 1 if first integration step; K ≠ 1 if other than first integration step	
LIMIT		Indicator: LIMIT < 10 if convergence occurs; LIMIT ≥ 10 if convergence criteria not satisfied	
N	n	Integration step size control	
REMAIN (I)	$(\xi_t)_{rem}$	Fraction of mass remaining in element i after convergence criteria satisfied	
R1LST	$(R_1)_{LST}$	Forward reaction rate for the first kinetic reaction for an element at mean primary zone mixture ratio (See Volume 2, Section 2 or Ref 3)	gm-mole/cm^3-sec
R6LST	$(R_6)_{LST}$	Forward reaction rate for the sixth kinetic reaction for an element at mean primary zone mixture ratio (See Volume 2, Section 2 or Ref 3)	gm-mole/cm^3-sec
STORE1		Dummy variable	gm-mole/cm^3-sec

Fortran Symbol	Symbol	Description	Units
STORE2		Dummy variable	gm-mole/ cm^3-sec
STORE3		Dummy variable	
STORE4		Dummy variable	
SUMT (I)	Σ_t	Sum to time t of the mass fractions in an element i	
SUMTNO (I)	Σ_{t-NO}	Sum to time t of the products of the mass fraction and NO concentrations in an element i	
TD	t_D	Time at end of integration interval	sec
TIMEN	t_n	Characteristic time used to calculate $(\xi_t)_D$	sec
TT	tt	Dummy variable	sec
TTS	tt_s	Time at end of integration interval	sec
TTU	tt_U	Time at start of integration interval	sec
TU	t_U	Time at start of integration interval	sec
YCH2XD	$[CH_2]_{e,x_D}$	Equilibrium mole fraction of unburned hydrocarbons exclusive of $C_{(s)}$ and CO for an element at the mean primary zone mixture ratio	
YCOXD	$[CO]_{e,x_D}$	Equilibrium mole fraction of CO for an element at the mean primary zone mixture ratio	
YCSXD	$[C_{(s)}]_{e,x_D}$	Equilibrium mole fraction of $C_{(s)}$ for an element at the mean primary zone mixture ratio	
YNOXD	$[NO]_{e,x_D}$	Equilibrium mole fraction of NO for an element at the mean primary zone mixture ratio	

Analysis Procedure

The step-by-step procedure of Subroutine PRCALC is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Estimate $(\alpha_2)_i$ as:

$$(\alpha_2)_i = 0.5$$

2. Calculate $(\alpha_U)_i$ as:

$$(\alpha_U)_i = 0 \quad \text{if} \quad [NO_i^+] = 0$$

$$(\alpha_U)_i = \frac{[NO_d]}{[NO_i^+]_e} \quad \text{if} \quad [NO_i^+] \neq 0$$

Step 3 is performed only if the chemical reaction rate is not significant.

3. Go to step 10.
4. Using Subroutine PRRAT, calculate a value of time which corresponds to the estimate of $(\alpha_2)_i$
5. Calculate t_{err} as:

$$t_{err} = 1 - \frac{tt}{\tau}$$

Steps 6 and 7 are performed only if $|t_{err}| \geq 0.05$.

6. Reestimate $(\alpha_2)_i$

Step 7 is performed only if the number of iterations on $(\alpha_2)_i$ are less than 10.

7. Go to step 4 .
8. Calculate $(\alpha_\tau)_i$ as:

$$(\alpha_\tau)_i = (\alpha_2)_i$$

Step 9 is performed only if the number of iterations on $(\alpha_\tau)_i$ equal 10.

9. Write the value of α_2
10. If this is not the last element in the array, go to step 1.
11. Initialize n as:

$$n = 10$$

Step 12 is performed only if $(\Sigma m_i)_j = 0$.

12. Go to step 50.

Step 13 is performed only if the chemical reaction rate is not significant.

13. Go to step 50.

14. Calculate $(\Delta\alpha)_i$ and t_U as:

$$(\Delta\alpha)_i = (\alpha_\Delta)_i / n$$

$$t_U = 0$$

15. Calculate $(\alpha_D)_i$ as:

$$(\alpha_D)_i = (\alpha_U)_i + (\Delta\alpha)_i$$

Step 16 is performed only if $(\alpha_D)_i > 1.0$.

16. Recalculate $(\alpha_D)_i$ as:

$$(\alpha_D)_i = 1.0$$

Steps 17 through 27 are performed only if $S_o = 0$

17. Using Subroutine MINT, calculate $(R_1)_{LST}$
18. Using Subroutine MINT, calculate $(R_2)_{LST}$
19. Using Subroutine MINT, calculate $(K_1)_{LST}$
20. Using Subroutine MINT, calculate $(K_2)_{LST}$
21. Using Subroutine MINT, calculate $[NO]_{e,x_D}$
22. Using Subroutine MINT, calculate $\bar{\rho}$
23. Using Subroutine MINT, calculate $\bar{T}$
24. Using Subroutine MINT, calculate $[CO_2]_{e,x_D}$
25. Using Subroutine MINT, calculate $[CO]_{e,x_D}$
26. Using Subroutine MINT, calculate $[CH_2]_{e,x_D}$
27. Calculate $(NO)_{e,x_D}$ as:

$$(NO)_{e,x_D} = \frac{[NO]_{e,x_D} * 30.0 * P}{\bar{\rho} * \bar{T} * 82.057}$$

28. Using Subroutine PRRAT, calculate $(\alpha_D)_i$.

Step 29 is performed only if $S_o = 0$

29. Calculate Q as:

$$Q = 0$$

Steps 30 through 32 are performed only for the first integration step.

30. Calculate $(\xi_t)_U$ as:

$$(\xi_t)_U = 0$$

31. Reset $(\alpha_U)_i$ and t_U as:

$$(\alpha_U)_i = (\alpha_D)_i$$

$$t_U = tt$$

32. Go to step 15.

33. Calculate t_D as:

$$t_D = tt$$

34. Calculate t_n as:

$$t_n = \frac{1}{2}(t_U + t_D)$$

35. Calculate $(\xi_t)_D$ as:

$$(\xi_t)_D = 1 - \exp(-t_n/\bar{\tau})$$

36. Calculate $\xi_t, (\xi_t)_U, \varepsilon_t$ and $\varepsilon_{t\text{-}NO}$

37. Reset $(\alpha_U)_i$ and t_U as:

$$(\alpha_U)_i = (\alpha_D)_i$$

$$t_U = t_D$$

Step 38 is performed if the convergence criteria on $(\xi_t)_{rem}$ are not satisfied but those on $\varepsilon_{t\text{-}NO}$ are.

38. Go to step 45.

Step 39 is performed if $tt < 5\bar{\tau}$

39. Go to step 15.

Steps 40 through 42 are performed if the convergence criteria on $\varepsilon_{t\text{-}NO}$ are not satisfied.

40. If the number of iterations on $\varepsilon_{t\text{-}NO}$ equal 6 go to step 43.

41. Reset n as:

$$n = 2n$$

42. Go to step 14.

43. If the number of iterations on $\varepsilon_{t\text{-}NO}$ are equal to 6, write a diagnostic statement identifying element and the last two values of $\varepsilon_{t\text{-}NO}$

44. Calculate $(\Delta\alpha)_i$ as:

$$(\Delta\alpha)_i = 5(\Delta\alpha)_i$$

45. Calculate $(\xi_t)_{rem}$ as:

$$(\xi_t)_{rem} = 1 - \varepsilon_t$$

Step 46 is performed if $\varepsilon_{t-NO} < 10^{-5}$

46. Go to step 48.

Step 47 is performed only if the number of iterations on $(f_t)_{rem}$ are less than or equal to 20.

47. If convergence criteria on $(f_t)_{rem}$ are not satisfied, reset $(\Delta\alpha)_i$ as:

$$(\Delta\alpha)_i = (\Delta\alpha_1)_i$$

and go to step 15.

48. Calculate ε_{t-NO} and $[NO_i]$

49. Reset n as:

$$n = n/8$$

50. If this is not the last element in the array, go to step 12.

51. Return.

```
      SUBROUTINE PRCALC(FNOXG)
      REAL NO
      DIMENSION SUMTNC(50),DUMMY(50),SUMT(50),REMAIN(50),ALPHAT(50),ALPH
     1AU(50),ALPHAD(50)
      COMMON/DATA1/AIR(50),RR(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(
     150),ZP(70),CUMDIS(70),VP,RHO(50),BCON6(50),ATT(50),PPP,FNOXP,R1(50
     2),R6(50),EK1(50),EK2(50),A2,A3,XL,CN,BETA,S,PHIP,EKS,XEND,A1
      COMMON/OUT3/INDIC,NO(50),AVET,TAUBAR,RHOBAR,PHIBAR,IMAX,XD,
     1FBARD,XU,LEN,TAUINT,TAUDIL,VELOC
      COMMON/OUT4/CONGNO(50),DELMD(50),AREAD,ASLOPE,DMFUO,SLOPE(50),TSLO
     1PE,NOP(50),EKKD,DMFT,UDM(50),DDM(50),     FB(50),DMFUD,AIRO,DMFFED
     2,RSUBX,SIG,SIGZER,AVEMW,DMDDA(50),DMDDM(50),DMDDP(50),DMDDPP(50),F
     3PRIME(50),NOEGXD,ANO,AQQ,DIFNO(50),NOZERO(50),RDOT(50),E(50)
C****
C**** SET INDICES,INITIAL VALUES,ETC.
C****
      TTU = 0.0
      TTS=0.0
      DO 50 I = 1,50
      NO(I) = 0.0
   50 CONTINUE
      DO 1000 I =1,IMAX
      ALPHA2=0.5
      LIMIT = 0
      IF(CONGNO(I).EQ.0.0) ALPHAU(I) = 0.0
      IF(CONGNO(I).NE.0.0) ALPHAU(I) = FNOXG/CONGNO(I)
      IF(NOZERO(I).EQ.1) GO TO 1000
      ALPHA1 = ALPHAU(I)
      DALP=ALPHA1
C****
C**** CALCULATE THE VALUE OF ALPHA-TAU
C****
  100 TT = TTU
      LIMIT=LIMIT+1
      CALL PRRAT(ALPHA1,ALPHA2,TT,I)
      AAA=ALPHA2
      ERR=(1.0-(TT/TAUBAR))
      IF(ABS(ERR)-0.05) 300,200,200
  200 ALPHA2=AAA+(AAA-DALP)*(TAUBAR-TT)/(TT-TTS)
      IF(ALPHA2.LE.0.0) ALPHA2 = AAA/2.
      IF(ALPHA2.GT.1.0) ALPHA2=1.2*AAA
      IF(ALPHA2.GT.1.0) ALPHA2=0.998
      DALP=AAA
      TTS=TT
      IF(LIMIT.LT.10) GO TO 100
  300 ALPHAT(I)=ALPHA2
      IF(LIMIT.EQ.10)  WRITE(6,9997) ALPHA2,LIMIT
 1000 CONTINUE
C****
C**** BEGIN NO CALCULATIONS FOR THE ITH ELEMENT
C****
      N = 10
      EN = N
      DO 5000 I =1,IMAX
      NO(I) = ALPHAU(I)
      IF(DELMD(I).EQ.0.0) GO TO 4000
      IF(NOZERO(I).EQ.1) GO TO 4000
C****
C**** SET ADDITIONAL INDICES,INITIAL VALUES,ETC.
C****
```

```
      INDEX = 0
      J = 1
      JJ=1
      DUMMY(I) = 0.0
 1150 DALPHA=ALPHAT(I)/EN
      SUMTNO(I) = 0.0
      SUMT(I) = 0.0
      K = 0
      ALPHU=ALPHAU(I)
      TU=0.0
 1200 ALPHD=ALPHU+DALPHA
C****
C**** PRRAT OVERWRITTEN IF ALPHD.GT.0.99
C****
      IF(ALPHD.GT.1.0) ALPHD = 1.
      TT=TU
C****
C**** SPECIAL CASE S=0.0 IN PRIMARY ZONE
C****
      IF(S.NE.0.0) GO TO 1210
      CALL MINT(1,FBARD,35,FF,R1,R1LST)
      CALL MINT(1,FBARD,35,FF,R6,R6LST)
      CALL MINT(1,FBARD,35,FF,EK1,EK1LST)
      CALL MINT(1,FBARD,35,FF,EK2,EK2LST)
      CALL MINT(1,FBARD,35,FF,BCON6,YNOXD)
      CALL MINT(1,FBARD,35,FF,RHO,RHOBAR)
      CALL MINT(1,FBARD,35,FF,ATT,AVET)
      CALL MINT(1,FBARD,35,FF,BCON1,YCSXD)
      CALL MINT(1,FBARD,35,FF,BCON2,YCOXD)
      CALL MINT(1,FBARD,35,FF,CH2,YCH2XD)
      STORE1 = R1(I)
      STORE2 = R6(I)
      STORE3 = EK1(I)
      STORE4 = EK2(I)
      R1(I) = R1LST
      R6(I) = R6LST
      EK1(I) = EK1LST
      EK2(I) = EK2LST
      NOEQXD=YNOXD*30.0/(RHOBAR*AVET*82.057/PPP)
 1210 CALL PRRAT(ALPHU,ALPHD,TT,I)
      IF(S.NE.0.0) GO TO 1220
      R1(I) = STORE1
      R6(I) = STORE2
      EK1(I) = STORE3
      EK2(I) = STORE4
      AQQ=0.0
 1220 CONTINUE
      K = K+1
      IF(K.NE.1) GO TO 1251
      FTU=0.0
      ALPHU=ALPHD
      TU=TT
      GO TO 1200
 1251 TD=TT
      TIMEN=0.5*(TU+TD)
      FTD=1.0-EXP(-TIMEN/TAUBAR)
      FT=FTD-FTU
      FTU=FTD
      TU=TD
      ALPHU=ALPHD
```

```
      SUMT(I) = SUMT(I)+FT
      SUMTNO(I)=SUMTNO(I)+ALPHU*CONGNO(I)*FT
      IF(INDEX.EQ.1) GO TO 1400
      IF(TT.LT.5.0*TAUBAR) GO TO 1200
      IF(ABS((SUMTNO(I)-DUMMY(I))/SUMTNO(I)).LE.0.01 ) GO TO 1300
      IF(J.EQ.6) GO TO 1300
      EN = 2.0*EN
      DUMMY(I) = SUMTNO(I)
      J = J+1
      GO TO 1150
 1300 IF(J.NE.6) GO TO 1350
      WRITE(6,9000) SUMTNO(I),DUMMY(I),I
 9000 FORMAT(55H POTENTIAL ERROR DUE TO LACK OF CONVERGENCE,SUMTNO(I)= ,
     1E15.8,2X,26HPRIOR VALUE OF SUMTNO(I)= ,E15.8,2X,3HI= ,I2///)
 1350 DALPHA=5.0*DALPHA
 1400 REMAIN(I) = 1.-SUMT(I)
      IF(REMAIN(I)*CONGNO(I) .GT.0.001*SUMTNO(I)) INDEX = 1
      IF(SUMTNO(I).LT.1.0E-05) GO TO 1500
      JJ=JJ+1
      IF(JJ.GT.20) GO TO 1500
      IF(REMAIN(I)*CONGNO(I) .GT.0.001*SUMTNO(I)) DALPHA=ALPHAT(I)
      IF(REMAIN(I)*CONGNO(I) .GT.0.001*SUMTNO(I)) GO TO 1200
 1500 SUMTNO(I)=SUMTNO(I)+(CONGNO(I)*ALPHU*REMAIN(I))
      NO(I) = SUMTNO(I)
      EN=EN/8.
 4000 CONTINUE
 5000 CONTINUE
 9997 FORMAT(35X,E12.5,I6)
      RETURN
      END
```

APPENDIX VIII - SUBROUTINE PRRAT

The function of Subroutine PRRAT is to solve the analytical expression relating nitric oxide concentration to time.

Subroutine PRRAT is called by Subroutine PRCALC; it does not call any other subroutines. Subroutine PRRAT does not require external input and does not provide external output. Internal input and output are transmitted through COMMON and as arguments of the subroutine. The internal input consists of:

CONGNO	EK1	EK2	FINIS	I
INIT	R1	R6	RHO	TIME

The internal output consists of:

TIME

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols in Subroutine PRRAT which are not included in COMMON:

Fortran Symbol	Symbol	Description	Units
A	A	Constant	cm^3/gm-mole
B	B	Constant	gm-mole/cm^3-sec
D	D	Constant	gm-mole/cm^3-sec
DUMMY	C_1	Dummy variable	cm^3-sec/gm-mole
DUMMYA	C_2	Dummy variable	cm^3-sec/gm-mole
DUMMYB	C_3	Dummy variable	
E	E	Constant	gm-mole/cm^3-sec
FINIS	$(\alpha_{fin})_i$	Ratio of NO concentration to NO concentration at equilibrium for an element of mixture ratio F and pressure P at the end of the integration interval	

Fortran Symbol	Symbol	Description	Units
I	i	Index of the element in question	
INIT	$(\alpha_{init})_i$	Ratio of NO concentration to NO concentration at equilibrium for an element of mixture ratio F and pressure P at the start of the integration interval	
TIME	t_o and t_f	Value of time at start of integration interval (t_o) and at end of integration interval (t_f)	sec

Analysis Procedure

The step-by-step procedure of Subroutine PRRAT is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. If $(\alpha_{fin})_i$ is greater than 0.39, then $t_f = 10 t_c$. Go to step 10.
2. Calculate A = $\dfrac{2 M_{NO}}{\rho_i [NO_i^{t}]_e}$
3. Calculate B = $\dfrac{(R_6)_i}{1 + (K_2)_i}$
4. Calculate D = $(R_1)_i + B$
5. Calculate E = $B * (K_1)_i$
6. Calculate C_1 = $\dfrac{E * (K_1)_i - D}{E^2 - D^2}$
7. Calculate C_2 = $\dfrac{E - (K_1)_i * D}{E^2 - D^2}$
8. Calculate C_3 = $\dfrac{[1 + (\alpha_{fin})_i][1 - (\alpha_{init})_i]}{[1 + (\alpha_{init})_i][1 - (\alpha_{fin})_i]}$
9. Calculate t_f = $t_o + \dfrac{1}{A} \left\{ \left[\frac{1}{2} C_1 \ln C_3 \right] + \left[C_2 \ln \left[\dfrac{(D + E*(\alpha_{fin})_i)(1 - (\alpha_{init})_i^2)^{1/2}}{(D + E*(\alpha_{init})_i)(1 - (\alpha_{fin})_i^2)^{1/2}} \right] \right] \right\}$
10. Return.

```
      SUBROUTINE PRRAT(INIT,FINIS,TIME,I)                               PRR*0000
      REAL INIT                                                         PRR*0010
      COMMON/DATA1/AIR(50),RH(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(PRR*0020
     150),ZP(70),CUMDIS(70),VP,RHO(50),BCON6(50),ATT(50),PPP,FNOXP,R1(50PRR*0030
     2),R6(50),EK1(50),EK2(50),A2,A3,XL,CN,BETA,S,PHIP,EKS,XEND,A1      PRR*0040
      COMMON/OUT4/CONGNO(50),DELMD(50),AREAD,ASLOPE,DMFUO,SLOPE(50),TSLOPRR*0050
     1PE,NOP(50),EKKD,DMFT,UDM(50),DDM(50),     FB(50),DMFUD,AIRD,DMFFEDPRR*0060
     2,RSUBX,SIG,SIGZER,AVEMW,DMDDA(50),DMDDM(50),DMDDP(50),DMDDPP(50),FPRR*0070
     3PRIME(50),NOEQXD,ANO,AQQ,DIFNO(50),NOZERO(50),RDOT(50),SUEA(50)   PRR*0080
C****                                                                   PRR*0090
C**** CALCULATE CONSTANTS                                               PRR*0100
C****                                                                   PRR*0110
      IF(FINIS.GT.0.99) GO TO 2000                                      PRR*0120
      A = (2.0*30.0)/(RHO(I)*CONGNO(I))                                 PRR*0130
      B = R6(I)/(1.+EK2(I))                                             PRR*0140
      D = R1(I)+B                                                       PRR*0150
      E = B*EK1(I)                                                      PRR*0160
      DUMMY = (E*EK1(I)-D)/(E*E-D*D)                                    PRR*0170
      DUMMYA = (E-EK1(I)*D)/(E*E-D*D)                                   PRR*0180
C****                                                                   PRR*0190
C**** CALCULATE TIME                                                    PRR*0200
C****                                                                   PRR*0210
      DUMMYB = ((1.+FINIS)*(1.-INIT))/((1.-FINIS)*(1.+INIT))            PRR*0220
      TIME = (1./A)*((0.5*DUMMY*ALOG(DUMMYB))+(DUMMYA*ALOG(((D+E*FINIS)*PRR*0230
     1SQRT(1.-INIT*INIT))/((D+E*INIT)*SQRT(1.-FINIS*FINIS)))))+TIME     PRR*0240
      GO TO 1000                                                        PRR*0250
 2000 TIME = 10.0*TIME                                                  PRR*0260
 1000 RETURN                                                            PRR*0270
      END                                                               PRR*0280
```

APPENDIX IX - SUBROUTINE MINT

The function of Subroutine MINT is to provide an interpolated value of a tabulated function of one variable assuming a linear, logarithmic, or exponential relationship.

Subroutine MINT is called by Subroutines PRCALC, ZINTER, DILUTE, CALCBC, and ZMASS; it does not call any other subroutines. Subroutine MINT does not require external input and does not provide external output. Internal input and output are transmitted as arguments of the subroutine. The internal input consists of:

ILN NTAB X XTAB YTAB.

The internal output consists of:

Y

Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols used in Subroutine MINT. Since the subroutine may be used with any consistent set of units, the units of the symbols are not specified.

Fortran Symbol	Symbol	Description	Units
A	a	Coefficient in the expression for Y as a function of X	
B	b	Coefficient in the expression for Y as a function of X	
ILN		Indicator: ILN=1 if linear interpolation is required ILN=2 if logarithmic interpolation is required ILN=3 if exponential interpolation is required	
N	n	Index of the tabular entry	
NTAB	N	Number of tabular entries	
N1	n_1	Index of the tabular entry preceding X	
N2	n_2	Index of the tabular entry following X	

Fortran Symbol	Symbol	Description	Units
X	X	Value of the independent variable at which interpolation is required	
XTAB(N)	$\hat{X}_n$	Tabular entries of the independent variable	
X1	X_{n_1}	Value of the independent variable at n_1	
X2	X_{n_2}	Value of the independent variable at n_2	
Y	Y	The value of the dependent variable to be interpolated	
YTAB(N)	$\hat{Y}_n$	Tabular entries of the dependent variable	
Y1	Y_{n_1}	Value of the dependent variable at n_1	
Y2	Y_{n_2}	Value of the dependent variable at n_2	

Analysis Procedure

The step-by-step procedure of subroutine MINT is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. If there is only one tabular entry, set $Y = Y_1$ and return.
2. If linear or logarithmic interpolation is specified, exclude extrapolation; that is,

   set $Y = Y_1$ if $X < X_1$

   set $Y = Y_n$ if $X > X_n$

   and return.
3. Determine the tabular entries n_1 and n_2 between which X lies.
4. Exclude those cases for which the interpolation formulas will degenerate, that is

   set $Y = \frac{1}{2}(Y_{n_1} + Y_{n_2})$ if $X_{n_1} = X_{n_2}$

   or, set $Y = Y_{n_1}$ if $Y_{n_1} = Y_{n_2}$
5. If linear interpolation is specified, set

$$Y = a + bX$$

where $a = Y_{n_1} - bX_{n_1}$

and $b = (Y_{n_2} - Y_{n_1})/(X_{n_2} - X_{n_1})$

and return.

6. If logarithmic interpolation is specified, set

$$Y = e^{a+b/X}$$

where
$$a = \ln(Y_{n_1}) - b/X_{n_1}$$

and
$$b = \ln(Y_{n_2}/Y_{n_1})/(1/X_{n_2} - 1/X_{n_1})$$

and return.

7. If exponential interpolation is specified; set

$$Y = a/X^b$$

where
$$a = Y_{n_1}(X_{n_1})^b$$

and
$$b = \ln(Y_{n_1}/Y_{n_2})/\ln(X_{n_2}/X_{n_1})$$

and return.

```
      SUBROUTINE MINT(ILN,X,NTAB,XTAB,YTAB,Y)

C     INTERPOLATION OF A FUNCTION OF ONE VARIABLE USING A MULTIPLICITY
C     OF METHODS

      DIMENSION XTAB(1),YTAB(1)

C     CHECK IF THERE IS ONLY ONE TABULAR ENTRY

      IF (NTAB.NE.1) GO TO 10
      Y=YTAB(1)
      RETURN

C     CHECK FOR EXTRAPOLATION IF  Y=A+B*X  OR  LN(Y)=A+B/X IS BEING USED

   10 IF (ILN.EQ.3) GO TO 50
      IF (X.GT.XTAB(1)) GO TO 20
      Y=YTAB(1)
      RETURN
   20 IF (X.LT.XTAB(NTAB)) GO TO 50
      Y=YTAB(NTAB)
      RETURN

C     FIND THE TABULAR ENTRIES BETWEEN WHICH X LIES

   50 DO 100 N=2,NTAB
      IF (X.GT.XTAB(N)) GO TO 100
      N2=N
      GO TO 200
  100 CONTINUE
      N2=NTAB
  200 N1=N2-1
      X1=XTAB(N1)
      X2=XTAB(N2)
      Y1=YTAB(N1)
      Y2=YTAB(N2)

C     CHECK FOR SPECIAL CASES

      IF (X1.NE.X2) GO TO 300
      Y=0.5*(Y1+Y2)
      RETURN
  300 IF (Y1.NE.Y2) GO TO 400
      Y=Y1
      RETURN
  400 GO TO (500,600,700),ILN

C     INTERPOLATE FOR Y USING   Y=A+B*X

  500 B=(Y2-Y1)/(X2-X1)
      A=Y1-B*X1
      Y=A+B*X
      RETURN

C     INTERPOLATE FOR Y USING   LN(Y)=A+B/X

  600 B=ALOG(Y2/Y1)/(1.0/X2-1.0/X1)
      A=ALOG(Y1)-B/X1
      Y=EXP(A+B/X)
      RETURN
```

```
C     INTERPOLATE FOR Y USING   Y=A/X**B

  700 B=ALOG(Y1/Y2)/ALOG(X2/X1)
      A=Y1*X1**B
      Y=A/X**B
      RETURN
      END
```

APPENDIX X - SUBROUTINE CALCBC

The function of Subroutine CALCBC is to calculate the value of the mass flow coefficient at each axial station in the combustor primary and intermediate zones.

Subroutine CALCBC is called by Subroutine ZMASS; it, in turn, calls Subroutine MINT. Subroutine CALCBC does not require external input and does not provide external output. Internal input and output are transmitted as arguments of the subroutine and through COMMON. The internal input consists of:

CUMDIS	MSTARD	ZP	ZPD

The internal output consists of:

C

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols in Subroutine CALCBC which are not included in COMMON.

Fortran Symbol	Symbol	Description	Units
C	C_{X_D}	Mass flow coefficient	gm/sec
P1	P_1	Value of the cumulative normal distribution at Zp	
P2	P_2	Value of the cumulative normal distribution at -Zp	
ZPD	Z_p	Limit of integration of the cumulative normal distribution	

Analysis Procedure

The step-by-step procedure of Subroutine CALCBC is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Using Subroutine MINT, calculate P_1
2. Calculate P_2 as :

$$P_2 = 1 - P_1$$

3. Calculate CX_D as:

$$C_{X_D} = \dot{m}_D^* / (P_1 - P_2)$$

4. Return:

```
      SUBROUTINE CALCBC(ZPD,C)
      REAL MSTARD,MSTARU
      COMMON/DATA1/AIR(50),RR(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(
     150),ZP(70),CUMDIS(70),VP,RHO(50),BCON6(50),ATT(50),PPP,FNOXP,R1(50
     2),R6(50),EK1(50),EK2(50),A2,A3,XL,CN,BETA,S,PHIP,EKS,XEND,A1
      COMMON/OUT5/MSTARD,MSTARU
      CALL MINT(1,ZPD,70,ZP,CUMDIS,P1)
      P2 = 1.0-P1
      C = MSTARD/(P1-P2)
      RETURN
      END
```

APPENDIX XI - SUBROUTINE CHECKK

The function of Subroutine CHECKK is to calculate the proportionality constant between the mass flow rate out of an element due to mixing and the total mass flowing into it. Subroutine CHECKK is called by Subroutine ZINTER; it does not call any other subroutines. Subroutine CHECKK does not require external input and does not provide external output. Internal input and output are transmitted as arguments of the subroutine and through COMMON. The internal input consists of:

A2	A3	CN	DELX	DMFUO
IMAX	MSTARU	SLOPE	UDM	XD
XL	XU			

The internal output consists of:

E	EKKD	RDOT

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols in Subroutine CHECKK which are not included in COMMON.

Fortran Symbol	Symbol	Description	Units
DELX	δx	Integration interval	cm
DUMMYA	φ_L	Dummy variable	cm^{-1}
RDOTT	$\dot{R}_T$	Total rate of change of unburned fuel with axial position in the combustor	gm/sec-cm

Analysis Procedure

The step-by-step procedure of Subroutine CHECKK is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Calculate K_D as:

$$K_D = C_N / X_L$$

2. Calculate $\dot{R}_T$ as:

$$\dot{R}_T = (\dot{m}_{FU_0})(A_3)\left[\left(\frac{X_D}{X_L}\right)^{A_2} - \left(\frac{X_U}{X_L}\right)^{A_2}\right] / \delta x$$

3. For the element in question, calculate E_i and $\dot{R}_i$ as:

$$E_i = K_D$$

$$\dot{R}_i = \dot{R}_T + (\delta m_i)_v / m_v^*$$

Step 4 is performed only if $(\delta m_i)_v = 0$

4. Go to step 7.

5. Calculate φ_i as:

$$\varphi_i = -\left[\frac{\partial(\delta m_i)_v}{\partial x} - \dot{R}_i\right] / (\delta m_i)_v$$

Step 6 is performed only if $\varphi_i \geq K_D$

6. Calculate E_i as:

$$E_i = 1.1\,\varphi_i$$

7. If this is the last element to be considered go to step 8. If not, return to step 3.

8. Return.

```
      SUBROUTINE CHECKK(DELX)
      REAL MSTARU
      DIMENSION DUMMYA(50)
      COMMON/DATA1/AIR(50),RR(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(
     150),ZP(70),CUMDIS(70),VP,RHO(50),BCON6(50),ATT(50),PPP,FNOXP,R1(50
     2),R6(50),EK1(50),EK2(50),A2,A3,XL,CN,BETA,S,PHIP,EKS,XEND,A1
      COMMON/OUT3/INDIC,NO(50),AVET,TAUBAR,RHOBAR,PHIBAR,IMAX,XD,
     1FBARD,XU,LEN,TAUINT,TAUDIL,VELOC
      COMMON/OUT4/CONGNO(50),DELMD(50),AREAD,ASLOPE,DMFUO,SLOPE(50),TSLO
     1PE,NOP(50),EKKD,DMFT,UDM(50),DDM(50),      FB(50),DMFUD,AIRD,DMFFED
     2,RSUBX,SIG,SIGZER,AVEMW,DMDDA(50),DMDDM(50),DMDDP(50),DMDDPP(50),F
     3PRIME(50),NOEQXD,ANO,AQQ,DIFNO(50),NOZERO(50),RDOT(50),E(50)
      COMMON/OUT5/MSTARD,MSTARU
C****
C**** CALCULATE K
C****
      EKKD=CN/XL
C****
C**** CHECK K VALUE
C****
      RDOTT = DMFUO*A3*(((XD/XL)**A2)-((XU/XL)**A2))/DELX
      DO 1000 I=1,IMAX
      E(I)=EKKD
      RDOT(I) = RDOTT*UDM(I)/MSTARU
      IF(UDM(I).EQ.0.0) GO TO 1000
      DUMMYA(I) = -(SLOPE(I)-RDOT(I))/UDM(I)
      IF(DUMMYA(I).GE.EKKD) E(I)=1.1*DUMMYA(I)
 1000 CONTINUE
      RETURN
      END
```

APPENDIX XII - SUBROUTINE RUNKUT

The function of Subroutine RUNKUT is to obtain the solution of a first-order ordinary differential equation by the Gill variation of the Runge-Kutta method.

Subroutine RUNKUT is called by Subroutine ZINTER and DILUTE; it, in turn, calls Subroutine DERIV. The subroutine does not require external input and does not provide external output. Internal input and output are transmitted as arguments of the subroutine. The internal input consists of:

DELX	I	LSGN	Q	XD
Y				

The internal output consists of:

Q	XU	Y

Fortran Nomenclature for Subroutine RUNKUT

The following table gives the Fortran nomenclature for those symbols used in Subroutine RUNKUT. Since the subroutine may be used with any consistent set of units, the units of the symbols are not specified. The subscript K, where it appears, is the index of the step in the Runge-Kutta solution.

Fortran Symbol	Symbol	Description	Units
A(K)	a_i	A set of constants used to determine DIFF	
B(K)	b_i	A set of constants used to determine DIFF	
C(K)	c_i	A set of constants used to determine Q	
D(K)	d_i	A set of constants used to determine X	
DELX	h	Increment in the independent variable across which the differential equation is to be solved	

Fortran Symbol	Symbol	Description	Units
DELY	k_i	Product of YPRIME and DELX at each stage of the solution	
DIFF	ΔY	The change in the value of the dependent variable at each stage of the solution	
I		Index of element	
K	I	Index of the stage of the solution	
LSGN		Indicator: LSGN=1 if intermediate zone and not the last step in the zone; LSGN=2 if intermediate zone and the last step in the zone; LSGN=3 if dilution zone or dilution zone type calculation	
Q	q_i	Quantity used to calculate DIFF at each stage of the solution; the value of Q in the final stage of the solution is a measure of the round-off error in Y	
X	X_i	Value of the independent variable at each stage of the solution	
Y	Y_i	Value of the dependent variable at each stage of the solution	
YPRIME	$f(X_i, X_i)$	Value of dY/dX at each stage of the solution	

Analysis Procedure

The step-by-step procedure of Subroutine RUNKUT is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Calculate the value of the independent variable at the given stage i of the solution as

$$X_i = X_{i-1} + (d_i)(h)$$

2. Using Subroutine DERIV, calculate the value of $f(X_i, Y_i)$ at the given stage of the solution.

3. Calculate k_i at the given stage of the solution as:

$$k_i = [f(x_i, Y_i)][h]$$

4. Calculate the change in the dependent variable at the given stage of the solution as:

$$\Delta Y = a_i + (k_i - b_i)(q_i)$$

5. Calculate the value of the dependent variable at the given stage of the solution as:

$$Y_i = Y_{i-1} + \Delta Y$$

Step 6 is performed only if $Y_i < 0$. If $Y_i \geq 0$ go to step 7.

6. Set $Y_i = 0$.
7. Calculate q_i as:

$$q_i = q_{i-1} + 3(\Delta Y) - (c_i)(k_i)$$

8. If this is the last stage of the solution, go to step 9. If not, return to step 1.
9. Return .

```
      SUBROUTINE RUNKUT(X,DELX,Y,Q,LSGN,I)
      DIMENSION A(4),B(4),C(4),D(4)
      DATA (A(I),I=1,4)/0.5,0.2928932,1.7071068,0.1666667/,(B(I),I=1,4)
     1/2.0,1.0,1.0,2.0/,(C(I),I=1,4)/0.5,0.2928932,1.7071068,0.5/,
     2(D(I),I=1,4)/0.0,0.5,0.0,0.5/
C****
C**** RUNKUT - SOLUTION OF A FIRST ORDER ORDINARY DIFFERENTIAL EQUATION
C****          BY THE GILL VARIATION OF THE RUNGE-KUTTA METHOD
C****
      DO 100 K=1,4
      X = X+D(K)*DELX
      CALL DERIV(X,Y,YPRIME,LSGN,I)
      DELY = YPRIME*DELX
      DIFF = A(K)*(DELY-B(K)*Q)
      Y = Y+DIFF
      IF(Y.LT.0.0)  Y=0.0
  100 Q = Q+3.0*DIFF-C(K)*DELY
      RETURN
      END
```

APPENDIX XIII - SUBROUTINE DERIV

The function of Subroutine DERIV is to calculate the rate of formation of nitric oxide with respect to axial distance in the combustor intermediate or dilution zone.

Subroutine DERIV is called by Subroutine RUNKUT; it does not call any other subroutines. Subroutine DERIV does not require external input and does not provide external output. Internal input and output are transmitted as arguments of the subroutine and through COMMON. The internal input consists of:

AREAD	ASLOPE	CONGNO	DDM
DMDDP	E	EK1	EK2
FNOXP	I	LSGN	MSTARD
NO	NOEQXD	NOP	NOZERO
RDOT	R1	R6	SLOPE
UDM	XD	Y	

The internal output consists of:

DILL	REAT	YPRIME

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols in Subroutine DERIV which are not included in COMMON.

Fortran Symbol	Symbol	Description	Units
DFLAME	$(\dot{r})_{Flame}$	Rate of change of elemental NO concentration with axial position in the combustor intermediate zone due to formation of "prompt NO"	cm^{-1}
DMIXT	$(\dot{r}_{mix})_{TOT}$	Total rate of change of elemental NO concentration with axial position in the combustor intermediate zone due to mixing	cm^{-1}

Fortran Symbol	Symbol	Description	Units
DMIX1	$(\dot{r}_{MIX})_1$	Rate of change of elemental NO concentration with axial position in the combustor intermediate zone due to mixing into the element	cm^{-1}
DMIX2	$(\dot{r}_{MIX})_2$	Rate of change of elemental NO concentration with axial position in the combustor intermediate zone due to mass change mixing term	cm^{-1}
DMIX3	$(\dot{r}_{MIX})_3$	Rate of change of elemental NO concentration with axial position in the combustor intermediate zone due to mixing out of the element	cm^{-1}
FNOXG	$[NO_o]$	NO formed in the flame front (mass fraction)	
I	i	Index of element	
LSGN		Indicator: LSGN=1 if intermediate zone and not the last step in the zone; LSGN=2 if intermediate zone and the last step in the zone; LSGN=3 if dilution zone or dilution zone type calculation	
RAT	$\begin{cases}(\alpha_D)_i \\ (\alpha_D)\end{cases}$	Ratio of NO concentration to NO concentration at equilibrium for an element of mixture ratio F and pressure P at axial position X_D; ratio of NO concentration to NO concentration at equilibrium at axial position X_D	
X	X_D	Axial position (downstream) in the combustor	cm
Y	$\begin{cases}[NO_i]_{X_D} \\ [\overline{NO}]_{X_D}\end{cases}$	Nitric oxide concentration for an element of mixture ratio F and pressure P (mass fraction) at X_D; nitric oxide concentration at X_D	

Fortran Symbol	Symbol	Description	Units
YPRIME	$\left\{\begin{array}{l}\left[\frac{\partial [NO_i]}{\partial x}\right]_{x_D} \\ \left[\frac{\partial [\bar{NO}]}{\partial x}\right]_{x_D}\end{array}\right.$	Rate of change of elemental NO concentration with axial position in the combustor intermediate zone; rate of change of NO concentration with axial position in the combustor dilution zone	cm^{-1}

Analysis Procedure

The step-by-step procedure of Subroutine DERIV is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Calculate $[NO_e]$

Steps 2 through 5 are performed only in the dilution zone or for a dilution zone type calculation.

2. If $[\bar{NO}_e]_{x_D} = 0$, then calculate $\left[\frac{\partial [\bar{NO}]}{\partial x}\right]_{x_D}$ as:

$$\left[\frac{\partial [\bar{NO}]}{\partial x}\right]_{x_D} = 0$$

3. If $[\bar{NO}_e]_{x_D} = 0$, go to step 18.
4. Calculate (α_D) as:

$$(\alpha_D) = \frac{[\bar{NO}]_{x_D}}{[\bar{NO}_e]_{x_D}}$$

5. Go to step 9.
6. Calculate $\left[\frac{\partial [NO_i]}{\partial x}\right]_{x_D}$ as:

$$\left[\frac{\partial [NO_i]}{\partial x}\right]_{x_D} = 0$$

Step 7 is performed only if $[NO_i^*]_e = 0$ or if the chemical reaction rate is not significant.

7. Go to step 18.
8. Calculate $(\alpha_D)_i$ as:

$$(\alpha_D)_i = \frac{[NO_i]}{[NO_i^*]_e}$$

9. Calculate $(\dot{r})_{react}$.

Steps 10 through 13 are performed in the intermediate zone except for the last step in the zone.

10. Calculate $(\dot{r}_{mix})_1$, $(\dot{r}_{mix})_2$, $(\dot{r}_{mix})_3$ and $(\dot{r})_{flame}$.

11. Calculate $(\dot{r}_{mix})_{TOT}$ as:

$$(\dot{r}_{mix})_{TOT} = (\dot{r}_{mix})_1 - (\dot{r}_{mix})_2 - (\dot{r}_{mix})_3 + (\dot{r})_{flame}$$

12. Calculate $\left[\frac{\partial [NO_i]}{\partial x}\right]_{x_D}$ as:

$$\left[\frac{\partial [NO_i]}{\partial x}\right]_{x_D} = (\dot{r}_{mix})_{TOT} + (\dot{r})_{react}$$

13. Go to step 18.

Steps 14 and 15 are performed only for the last step in the intermediate zone.

14. Calculate $\left[\frac{\partial [NO_i]}{\partial x}\right]_{x_D}$ as:

$$\left[\frac{\partial [NO_i]}{\partial x}\right]_{x_D} = (\dot{r})_{react}$$

15. Go to step 18 .

Steps 16 and 17 are performed in the dilution zone or for a dilution zone type calculation.

16. Calculate $(\dot{r})_{DIL}$

17. Calculate $\left[\frac{\partial [\overline{NO}]}{\partial x}\right]_{x_D}$ as:

$$\left[\frac{\partial [\overline{NO}]}{\partial x}\right]_{x_D} = (\dot{r})_{react} + (\dot{r})_{DIL}$$

18. Return .

```
      SUBROUTINE DERIV(X,Y,YPRIME,LSGN,I)
      REAL MSTARD,MSTARU,NOP,NOEQXD,NO
      COMMON/DATA1/AIR(50),RR(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(
     150),ZP(70),CUMDIS(70),VP,RHO(50),BCON6(50),ATT(50),FOP,FNOXP,R1(50
     2),R6(50),EK1(50),EK2(50),A2,A3,XL,CN,BETA,S,PHIP,EKS,XEND,A1
      COMMON/OUT3/INDIC,NO(50),AVET,TAUBAR,RHOBAR,PHIBAR,IMAX,XD,
     1FBARD,XU,LEN,TAUINT,TAUDIL,VELOC
      COMMON/OUT4/CONGNO(50),DELMD(50),AREAD,ASLOPE,DMFUO,SLOPE(50),TSLO
     1PE,NOP(50),EKKD,DMFT,UDM(50),DDM(50),     FB(50),DMFUD,AIRD,DMFFED
     2,RSUBX,SIG,SIGZER,AVEMW,DMDDA(50),DMDDM(50),DMDDP(50),DMDDPP(50),F
     3PRIME(50),NOEQXD,ANO,AQQ,DIFNO(50),NOZERO(50),RDOT(50),E(50)
      COMMON/OUT5/MSTARD,MSTARU
      COMMON/OUT6/REAT,DILL
      FNOXG = FNOXP*1.0E-06*(30.0/28.0)
      IF(LSGN.NE.3) GO TO 500
      IF(NOEQXD.EQ.0.0) YPRIME = 0.0
      IF(NOEQXD.EQ.0.0) GO TO 4000
      RAT = Y/NOEQXD
      GO TO 750
  500 CONTINUE
      YPRIME=0.0
      IF(CONGNO(I).EQ.0.0.OR.NOZERO(I).EQ.1) GO TO 4000
      RAT = Y/CONGNO(I)
  750 CONTINUE
      YPRIME=(((2.0*30.0)/(MSTARD/AREAD))*(1.0-RAT*RAT)*((R1(I)/(1.0+(RA
     1T*EK1(I))))+(R6(I)/(1.0+EK2(I)))))
      REAT = YPRIME
      GO TO (1000,2000,3000),LSGN
 1000 DMIX1=(DMDDP(I)+RDOT(I))*NOP(I)
      DMIX2=E(I)*UDM(I)*NO(I)
      DMIX3=SLOPE(I)*NO(I)
      DFLAME = FNOXG*RDOT(I)
      DMIXT = DMIX1-DMIX2-DMIX3+DFLAME
      DMIXT=DMIXT/DDM(I)
      YPRIME = DMIXT+REAT
      GO TO 4000
 2000 YPRIME = REAT
      GO TO 4000
 3000 DILL = -(Y/MSTARD)*ASLOPE
      YPRIME=YPRIME+DILL
 4000 RETURN
      END
```

APPENDIX XIV - SUBROUTINE ZMASS

The function of Subroutine ZMASS is to determine the mass flow in each element of the distribution function at a prescribed axial station in a gas turbine combustor. In addition, ZMASS calculates the mean mixture ratio, total mass flow, and the airflow rate at each of these axial stations.

Subroutine ZMASS is called by Subroutines PRIMRY, ZINTER, and DILUTE; it, in turn, calls Subroutines CALCBC and MINT. The subroutine does not require external input but does provide external output. Internal input and output are transmitted as arguments of the subroutine and through COMMON. The internal input consists of:

AIR	A1	A2	A3	BETA
CUMDIS	DDM	DELX	EKS	FF
INDIC	MSTARD	PHIP	PPP	RR
S	VP	XD	XL	XU
XX	ZP			

The internal output consists of:

AIRD	AREAD	ASLOPE	DDM	DELMD
DMFFED	DMFT	DMFUD	DMFUO	FB
FBARD	IMAX	MSTARD	MSTARU	NOZERO
SIG	SIGZER	SLOPE	TSLOPE	UDM

The external output consists of:

AFR	DDM	FEDF	FULOAD	IHIGHD
ILOWD				

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols used in Subroutine ZMASS which are not included in COMMON.

Fortran Symbol	Symbol	Description	Units
A	A	Lower integration limit for the evaluation of the cumulative normal distribution integral	

Fortran Symbol	Symbol	Description	Units
ADDM	$(\delta m)_A$	Dummy variable	gm/sec
AFR	A/F	Over-all air-to-fuel ratio	
AIRI	$(\dot{M}_A)_I$	Airflow rate at the primary zone exit	gm/sec
AIRU	$(\dot{M}_A)_{X_U}$	Airflow rate at the upstream axial integration limit of the combustor	gm/sec
B	B	Upper integration limit for the evaluation of the cumulative normal distribution integral	
C	C_{X_D}	Mass flow coefficient	gm/sec
DELX	δX	Increment of the combustor length across which the solution is generated	cm
DUMMY	$(FB)_{DUM}$	Dummy variable	
FEDF	$(\dot{M}_f)_f$	Total mass of fuel fed into the combustor	lb/hr; lb/sec
FJLOAD	ψ	Fuel loading	lb/sec-ft^3-atm^2
I	i	Index of the element	
IHIGHD	$(I_{HIGH})_D$	Subscript of the mass element with the highest equivalence ratio (downstream end of integration interval)	
IHIGHU	$(I_{HIGH})_U$	Subscript of the mass element with the highest equivalence ratio (upstream end of integration interval)	
ILOWD	$(I_{LOW})_D$	Subscript of the mass element with the lowest equivalence ratio (downstream end of integration interval)	
ILOWU	$(I_{LOW})_U$	Subscript of the mass element with the lowest equivalence ratio (downstream end of integration interval)	
IN		Counter; indicates first mass element with zero mass at upper end of equivalence ratio distribution function	
KKOUNT	K_{KOUNT}	Indicator KKOUNT = 0 if FB(I) $\leq 2\bar{F}$ for the element i KKOUNT = 1 if FB(I) $> 2\bar{F}$ for the element i	

Fortran Symbol	Symbol	Description	Units
KOUNT	K_{COUNT}	Indicator KOUNT = 0 if the element i has no mass KOUNT = 1 if the element i contains mass	
NN	N_n	Number of elements in the array	
NNN	N_{nn}	Number of last mixture ratio boundary	
NPRINT		Indicator NPRINT = 0 if intermediate output is not requested by the user NPRINT = 1 if intermediate output is re--quested by the user	
PI	π	Constant - equal to 3.14159265	
P1	P_1	Value of the normal distribution integral from $-\infty$ to A	
P2	P_2	Value of the cumulate normal distribution integral from $-\infty$ to B	
SDDM	$\Sigma \delta \dot{m}_i$	Sum of the element mass flows	gm/sec
ZPD	Z_{PX_D}	Limit of integration of the cumulative normal distribution	

Analysis Procedure

The step-by-step procedure of Subroutine ZMASS is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

Step 1 is performed only for the primary zone.

1. Calculate $(I_{LOW})_D$ and $(I_{HIGH})_D$ as:
   $(I_{LOW})_D = 0$
   $(I_{HIGH})_D = 50$
2. Calculate $(I_{LOW})_U$ and $(IHIGH)_U$ as:
   $(I_{LOW})_U = (I_{LOW})_D$
   $(I_{HIGH})_U = (I_{HIGH})_D$
3. Initialize N_n
4. Calculate N_{nn} as:
   $N_{nn} = N_n + 1$

5. Initialize $\Sigma \delta m_i$ as:

$$\Sigma \delta m_i = 0$$

6. Using Subroutine MINT, calculate $(\dot{M}_A)_I$
7. Using Subroutine MINT, calculate $(\dot{M}_A)_{X_U}$
8. Using Subroutine MINT, calculate $M_A|_{X_D}$
9. Using Subroutine MINT, calculate R_{X_D}
10. Calculate A X_D as:

$$A|_{X_D} = \pi R_{X_D}^2$$

11. Calculate $(\dot{M}_f)_{fed}$ as:

$$(\dot{M}_f)_{fed} = k_s * \bar{\phi}_p * (\dot{M}_A)_I / \beta$$

Step 12 is only performed in the intermediate and dilution zones.

12. Calculate the fuel loading, ψ as:

$$\psi = (\dot{M}_f)_{fed} * 12^3 * 2.54^3 / (454 * V_P * P^2)$$

Step 13 is performed only in the intermediate zone and if $M_U^* = 0$.

13. Write the fuel loading, ψ .
14. Calculate $(\dot{M}_f)_o$ and $(\dot{M}_f)_f$ as

$$(\dot{M}_f)_o = (\dot{M}_f)_f * (1 - \beta)$$

$$(\dot{M}_f)_f = (\dot{M}_f)_{fed} * 454$$

15. Calculate the over-all air-to-fuel ratio A/F as:

$$A/F = M_A|_{X_{END}} / (\dot{M}_f)_{fed}$$

16. Readjust the units on $(\dot{M}_f)_f$ from lb/sec to lb/hr.

Step 17 is only performed for the primary zone.

17. Write $(\dot{M}_f)_f$ and A/F.

Step 18 is performed only in the dilution zone.

18. Calculate $(\dot{M}_{fU})_{X_D}$ as:

$$(\dot{M}_{fU})_{X_D} = 0$$

Step 19 is performed only in the primary and intermediate zones.

19. Calculate $(\dot{M}_{fU})_{X_D}$ as:

$$(\dot{M}_{fU})_{X_D} = (\dot{M}_f)_o \left[1 - A_3\left(\frac{X_D}{X_L}\right)^{A_2}\right]$$

20. Calculate $(\dot{M}_F)_{X_D}$ as:

$$(\dot{M}_F)_{X_D} = (\dot{M}_F)_{Fed} - (\dot{M}_{FU})_{X_D}$$

21. Calculate M^*_U as:

$M^*_U = 0$ in the primary zone

$M^*_U = M^*_D$ in the intermediate and dilution zones

22. Calculate M^*_D as:

$$M^*_D = (\dot{M}_F)_{X_D} + M_A\big|_{X_D}$$

23. Calculate $\bar{F}$ as:

$$\bar{F} = \frac{(\dot{M}_F)_{X_D}}{M^*_D}$$

Step 24 is only performed in the primary zone.

24. Calculate σ_o as:

$$\sigma_o = S_o * \bar{F}$$

25. Calculate σ as:

$$\sigma = \sigma_o \left[1 - \left(\frac{X_D}{X_L}\right)^{A_1}\right]$$

Steps 26 and 27 are performed only in the dilution zone:

26. Recalculate σ as:

$$\sigma = 0$$

27. Go to step 91.

Step 28 is performed only if $S_o = 0$.

28. Go to step 31.

29. Calculate $Z_{P_{X_D}}$ as:

$$Z_{P_{X_D}} = \bar{F}/\sigma$$

30. Using Subroutine CALCBC, calculate C_{X_D}.

Step 31 is performed only in the intermediate and dilution zones.

31. Go to step 36.

32. Calculate $(F_B)_1$ as:

$(F_B)_1 = 0$.

Step 33 is performed for each boundary i satisfying the criteria $2 \leq i \leq N_n$

33. Calculate $(F_B)_i$ as:

$$(F_B)_i = \frac{1}{2}(F_i + F_{i-1})$$

34. Calculate $(F_B)_{N_{nn}}$ as:

$$(F_B)_{N_{nn}} = 2 * F_{N_n} - (F_B)_{N_{nn}}$$

35. Go to step 41.

Steps 36 and 37 are perfoimed for each element i satisfying the criteria $1 \leq i \leq i_{MAX}$.

36. Calculate $(\delta m_i)_U$ as:

$(\delta m_i)_U = 0$ in the primary zone

$(\delta m_i)_U = (\delta m_i)_D$ in the intermediate and dilution zones

37. Calculate $(\Delta m_i)_D$ as:

$$(\Delta m_i)_D = 0$$

Step 38 is performed only if $i_{MAX} = N_n$

38. Go to step 41.

Steps 39 and 40 are performed for each element i in the array satisfying the criteria $(i_{MAX} + 1) \leq i \leq N_n$.

39. Calculate $(\Delta m_i)_D$ as:

$$(\Delta m_i)_D = 0$$

40. Calculate $(\delta m_i)_U$ as:

$$(\delta m_i)_U = 0$$

41. Calculate i_{MAX} as:

$i_{MAX} = 50$

Step 42 is performed only for the special case that $S_D = 0$ in the primary zone.

42. Go to step 44.

43. Go to step 49.

Steps 44 through 48 are performed for each element i in the array satisfying the criteria $1 \leq i \leq i_{MAX}$.

44. Calculate $(\delta m_i)_D$ and $(\Delta m_i)_D$ for the next element as:

$$(\delta m_i)_D = 0$$

$$(\Delta m_i)_D = 0$$

Step 45 is performed only if $(F_B)_i < \bar{F}$.

45. Go to step 44.
46. Recalculate i_{MAX} as:

$$i_{MAX} = i-1$$

47. Calculate $(\delta m_i)_D$ and $(\phi m_i)_D$ as:

$$(\delta m_i)_D = M_D^{*}$$
$$(\phi m_i)_D = M_D^{x}$$

48. Go to step 92.
49. Initialize the indicators K_{COUNT} and K_{KOUNT} as

$K_{COUNT} = 0$
$K_{KOUNT} = 0$

Steps 50-85 are performed for each element i in the array satisfying the criteria $2 \leq i \leq N_{nn}$.

Steps 50 and 51 are performed only if the element i is equal to N_{nn}.

50. Calculate i_{MAX} as:

$i_{MAX} = N_{nn}-1$

51. Go to step 75.

Step 52 is performed only if $(F_B)_i \leq 2\bar{F}$

52. Go to step 54.
53. Calculate $(F_B)_{DUM}$, $(F_B)_i$, i_{MAX}, and K_{KOUNT} as:

$$(F_B)_{DUM} = (F_B)_i$$
$$(F_B)_i = 2\bar{F}$$
$$i_{MAX} = i-1$$
$$K_{KOUNT} = 1$$

54. Calculate the distribution integration limits as:

$$A = [(F_B)_i - \bar{F}] / \sigma$$
$$B = [(F_B)_{i-1} - \bar{F}] / \sigma$$

Steps 55 and 56 are performed only if $A \geq 0$.

55. Using Subroutine MINT, calculate P_1, the value of the normal distribution integral from $-\infty$ to A.

56. Go to step 60.

57. Calculate A as:

$A = -A$

58. Using Subroutine MINT, calculate the value of the normal distribution integral from $-\infty$ to A .

59. Recalculate P_1 as

$P_1 = 1 - P_1$

Steps 60 and 61 are performed only if $B \geq 0$.

60. Using Subroutine MINT, calculate P_2, the value of the normal distribution integral from $-\infty$ to B.

61. Go to step 65.

62. Calculate B as:

$B = 1 - B$

63. Using Subroutine MINT, calculate P_2, the value of the normal distribution integral from $-\infty$ to B.

64. Recalculate P_2 as:

$P_2 = 1 - P_2$

65. Calculate $(\delta m_i)_D$ as:

$$(\delta m_i)_D = C_{x_D} * (P_1 - P_2)$$

Step 66 is performed only if $(\delta m_i)_D > 0$.

66. Set $(I_{LOW})_D$ equal to 1.

Step 67 is performed only if $(I_{LOW})_D > 0$.

67. Go to step 69.

Step 68 is performed only if $(\delta m_{i-2})_D = 0$ and $(\delta m_{i-1})_D > 0$.

68. Set $(I_{LOW})_D$ equal to i-1.

Step 69 is performed only if $(\delta m_{i-1})_D > 0$.

69. Reset K_{COUNT} as:

$K_{COUNT} = 1$

Step 70 is performed only if $(\delta m_{i-1})_D = 0$ and if $K_{COUNT} = 1$.

70. Go to step 77.

Step 71 is performed only if $(i-1) = i_{MAX}$.

71. Go to step 74.

72. Calculate $\Sigma \delta m_i$ as:

$$\Sigma \delta m_i = \Sigma \delta m_i + (\delta m_{i-1})_D$$

73. Go to step 83.

74. Calculate $(\delta m)_A$ as:

$$(\delta m)_A = (\delta m_{i-1})_D$$

75. Calculate $(\delta m_{i-1})_D$, $(\Delta m_{i-1})_D$, and $(I_{HIGH})_D$ as:

$$(\delta m_{i-1})_D = M^*_D - \Sigma \delta m_i$$

$$(\Delta m_{i-1})_D = (\delta m_{i-1})_D$$

$$(I_{HIGH})_D = i-1$$

76. Go to step 81.

77. Calculate $(\delta m_{i-2})_D$, $(\Delta m_{i-2})_D$ and $(\Delta m_{i-1})_D$ as:

$$(\delta m_{i-2})_D = m^*_D - \Sigma \delta m_i + (\delta m_{i-2})_D$$

$$(\Delta m_{i-2})_D = (\delta m_{i-2})_D$$

$$(\Delta m_{i-1})_D = 0$$

78. Caluclate $(I_{HIGH})_D$ and i_{MAX} as:

$$(I_{HIGH})_D = i-2$$

$$i_{MAX} = i-2$$

Step 79 is performed only if $K_{KOUNT} = 1$.

79. Calculate $(F_B)_{IMAX+2}$ as:

$$(F_B)_{IMAX+2} = (F_B)_{DUM}$$

80. Reset $K_{KOUNT} = 0$.

Step 81 is performed only if $i_{MAX} > N_{nn}$.

81. Go to step 85.

82. Go to step 86.

83. Calculate $(\Delta m_{i-1})_D$ as:

$$(\Delta m_{i-1})_D = (\delta m_{i-1})_D$$

Step 84 is performed only if $i_{MAX} < 50$.

84. Go to step 86.

85. If this is the last element in the array, continue to step 86. If not, return to step 50 with $i = i + 1$.

Steps 86-87 are performed only if intermediate output is requested by the user.

Step 86 is performed for each element in the array satisfying the criteria $1 \leq i \leq i_{MAX}$.

86. Write $(\delta m_i)_D$

87. Write $(I_{LOW})_D$ and $(I_{HIGH})_D$.

Step 88 is performed if $K_{KOUNT} = 1$.

88. Calculate $(F_B)_{i_{MAX}+1}$ as:

$$(F_B)_{i_{MAX}+1} = (F_B)_{DUM}$$

Step 89 is performed only in the primary zone.

89. Go to step 92.

Step 90 is performed for each element in the array satisfying the criteria $1 \leq i \leq i_{MAX}$

90. Calculate $\left[\frac{\partial(\delta m_i)}{\partial x}\right]_{X_D}$ as:

$$\left[\frac{\partial(\delta m_i)}{\partial x}\right]_{X_D} = \frac{(\delta m_i)_D - (\delta m_i)_U}{\delta x}$$

91. Calculate $\left[\frac{\partial \dot{m}_A}{\partial x}\right]_{X_D}$ and $\left[\frac{\partial \dot{m}^*}{\partial x}\right]_{X_D}$ as:

$$\left[\frac{\partial \dot{m}_A}{\partial x}\right]_{X_D} = \frac{(\dot{m}_A)_{X_D} - (\dot{m}_A)_{X_U}}{\delta x}$$

$$\left[\frac{\partial \dot{m}^*}{\partial x}\right]_{X_D} = \frac{\dot{m}^*_D - \dot{m}^*_U}{\delta x}$$

92. Return.

```
      SUBROUTINE ZMASS(DELX)
      REAL MSTARD,MSTARU
      COMMON/DATA1/AIR(50),RR(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(
     150),ZP(70),CUMDIS(70),VP,RHO(50),BCON6(50),ATT(50),PPP,FNOXP,R1(50
     2),R6(50),EK1(50),EK2(50),A2,A3,XL,CN,BETA,S,PHIP,EKS,XEND,A1
      COMMON/OUT3/INDIC,NO(50),AVET,TAUBAR,RHOBAR,PHIBAR,IMAX,XD,
     1FBARD,XU,LEN,TAUINT,TAUDIL,VELOC
      COMMON/OUT4/CONGNO(50),DELMD(50),AREAD,ASLOPE,DMFUO,SLOPE(50),TSLO
     1PE,NOP(50),EKKD,DMFT,UDM(50),DDM(50),      FB(50),DMFUD,AIRD,DMFFED
     2,RSUBX,SIG,SIGZER,AVEMW,DMDDA(50),DMDDM(50),DMDDP(50),DMDDPP(50),F
     3PRIME(50),NOEQXD,ANO,AQQ,DIFNO(50),NOZERO(50),RDOT(50),E(50)
      COMMON/OUT5/MSTARD,MSTARU
      DATA PI/3.14159265/
C****
C**** CALCULATE AIR FLOW AND COMBUSTOR AREA
C****
      NPRINT=0
      IF(INDIC.NE.1) GO TO 10
      ILOWD=0
      IHIGHD=50
   10 ILOWU=ILOWD
      IHIGHU=IHIGHD
      NN=35
      NNN=NN+1
      SDDM=0.0
      CALL MINT(1,0.0,11,XX,AIR,AIRI)
      CALL MINT(1,XU,11,XX,AIR,AIRU)
      CALL MINT(1,XD,11,XX,AIR,AIRD)
      CALL MINT(1,XD,11,XX,RR,RSUBX)
      AREAD = PI*RSUBX*RSUBX
C****
C**** CALCULATE FUEL FLOW RATES AND DISTRIBUTION CHARACTERISTICS
C****
      DMFFED = EKS*PHIP*AIRI/BETA
      IF(INDIC.NE.1) FULOAD=DMFFED*12.0**3.0*2.54**3.0/(454.*VP*PPP**2.)
      IF(INDIC.EQ.2.AND.MSTARU.EQ.0.0) WRITE(6,8500) FULOAD
 8500 FORMAT(/////,1X,20HTHE FUEL LOADING IS ,E12.5,28H LB./SEC.-CU.FT.-
     1ATMO.-ATMO.)
      DMFUO = DMFFED*(1.0-BETA)
      FEDF = DMFFED/454.
      AFR = AIR(11)/DMFFED
      FEDF = FEDF*3600.
      IF(INDIC.EQ.1) WRITE(6,9100) FEDF
      IF(INDIC.EQ.1) WRITE(6,9150) AFR
      IF(INDIC.EQ.3) DMFUD = 0.0
      IF(INDIC.EQ.3) GO TO 100
      DMFUD = DMFUO*(1.-A3* (XD/XL)**A2)
  100 DMFT = DMFFED-DMFUD
      IF(INDIC.EQ.1) MSTARU = 0.0
      IF(INDIC.NE.1) MSTARU = MSTARD
      MSTARD = DMFT+AIRD
      FBARD = DMFT/MSTARD
      IF(INDIC.EQ.1) SIGZER=S*FBARD
      SIG=SIGZER*(1.0-(XD/XL)**A1)
      IF(INDIC.EQ.3) SIG = 0.0
      IF(INDIC.EQ.3) GO TO 8000
      IF(S.EQ.0.0) GO TO 500
C****
C**** CALCULATE DISTRIBUTION CHARACTERISTICS AND C
C****
```

```
      ZPD = FBARD/SIG
      CALL CALCBC(ZPD,C)
C****
C**** CALCULATE BOUNDARIES AT WHICH EACH F VALUE APPLIES
C****
  500 CONTINUE
      IF(INDIC.NE.1) GO TO 1500
      FB(1) = 0.0
      DO 1000 I=2,NN
 1000 FB(I)=        0.5*(FF(I)+FF(I-1))
      FB(NNN)=2.0*FF(NN)-FB(NN)
      GO TO 3000
C****
C**** STORE MASS FLOWS AT PREVIOUS STATION
C****
 1500 CONTINUE
      DO 2000 I =1,IMAX
      IF(INDIC.EQ.1) UDM(I)= 0.0
      IF(INDIC.NE.1) UDM(I) = DDM(I)
      DELMD(I)=0.0
 2000 CONTINUE
      IF(IMAX.EQ.NN) GO TO 2200
      IN=IMAX+1
      DO 2100 I=IN,NN
      DELMD(I)=0.0
 2100 UDM(I) = 0.0
 2200 CONTINUE
C****
C**** CALCULATE IMAX
C****
 3000 CONTINUE
      IMAX=50
C****
C**** SPECIAL CASE S=0.0 IN PRIMARY ZONE
C****
      IF(S.EQ.0.0.AND.INDIC.EQ.1) GO TO 2300
      GO TO 2500
 2300 DO 2400 I=1,IMAX
      DDM(I)=0.0
      DELMD(I)=0.0
      NOZERO(I)=1
      IF(FB(I).LT.FBARD) GO TO 2400
      IMAX=I-1
      DDM(I-1)=MSTARD
      DELMD(I-1)=MSTARD
      NOZERO(I-1)=0
      GO TO 9000
 2400 CONTINUE
 2500 CONTINUE
      KOUNT=0
      KKOUNT=0
      DO 5000 I =2,NNN
      IF(I.EQ.NNN) IMAX=NNN-1
      IF(I.EQ.NNN) GO TO 4880
      IF(FB(I).LT.(2.0*FBARD)) GO TO 4000
      DUMMY = FB(I)
      FB(I) = 2.0*FBARD
      IMAX = I-1
      KKOUNT=1
 4000 CONTINUE
```

```
C****
C**** CALCULATE THE ELEMENT MASSES
C****
      A = (FB(I)-FBARD)/SIG
      B = (FB(I-1)-FBARD)/SIG
      IF(A.GE.0.0) CALL MINT(1,A,70,ZP,CUMDIS,P1)
      IF(A.GE.0.0) GO TO 4500
      A = -A
      CALL MINT(1,A,70,ZP,CUMDIS,P1)
      P1 = 1.0-P1
 4500 IF(B.GE.0.0) CALL MINT(1,B,70,ZP,CUMDIS,P2)
      IF(B.GE.0.0) GO TO 4800
      B=-B
      CALL MINT(1,B,70,ZP,CUMDIS,P2)
      P2 = 1.0-P2
 4800 DDM(I-1) = C*(P1-P2)
      IF(DDM(1).GT.0.0) ILOWD=1
      IF(ILOWD.GT.0)  GO TO 4850
      IF(DDM(I-2).EQ.0.0.AND.DDM(I-1).GT.0.0) ILOWD=I-1
 4850 IF(DDM(I-1).GT.0.0) KOUNT=1
      IF(DDM(I-1).EQ.0.0.AND.KOUNT.EQ.1) GO TO 4900
      IF((I-1).EQ.IMAX) GO TO 4875
      SDDM=SDDM+DDM(I-1)
      GO TO 4950
 4875 ADDM=DDM(I-1)
 4880 DDM(I-1)=MSTARD-SDDM
      DELMD(I-1)=DDM(I-1)
      IHIGHD=I-1
      GO TO 4925
 4900 DDM(I-2)=MSTARD-SDDM+DDM(I-2)
      DELMD(I-2) = DDM(I-2)
      DELMD(I-1)=0.0
      IHIGHD=I-2
      IMAX=I-2
      IF(KKOUNT.EQ.1)  FB(IMAX+2)=DUMMY
      KKOUNT=0
 4925 CONTINUE
      IF(IMAX.GT.NNN) GO TO 5000
      GO TO 6000
 4950 DELMD(I-1)=DDM(I-1)
      IF(IMAX.LT.50) GO TO 6000
 5000 CONTINUE
 6000 CONTINUE
      IF(NPRINT.EQ.1) WRITE(6,9999)(DDM(I),I=1,IMAX)
      IF(NPRINT.EQ.1) WRITE(6,9998) ILOWD,IHIGHD
      IF(KKOUNT.EQ.1) FB(IMAX+1) =DUMMY
C****
C**** CALCULATE SLOPES
C****
      IF(INDIC.EQ.1) GO TO 9000
      DO 7000 I =1,IMAX
      SLOPE(I) = (DDM(I)-UDM(I))/DELX
 7000 CONTINUE
 8000 CONTINUE
      ASLOPE = (AIRD-AIRU)/DELX
      TSLOPE = (MSTARD-MSTARU)/DELX
 9100 FORMAT(/////,10X,58HTHE COMPUTED TOTAL MASS OF FUEL FED INTO THE C
     1OMBUSTOR IS ,E12.5,8H LB./HR.///)
 9150 FORMAT(10X,42HTHE COMPUTED OVERALL AIR-TO-FUEL RATIO IS ,E12.5,///
     1)
```

```
9998 FORMAT(5X,20I5//)
9999 FORMAT(10X,10E10.3/ )
9000 RETURN
     END
```

APPENDIX XV - SUBROUTINE PRINTS

The function of Subroutine PRINTS is to provide the written output of the calculated results of the program.

Subroutine PRINTS is called by Subroutines PRIMRY, ZINTER, and DILUTE; it does not call any other subroutine. Subroutine PRINTS does not require external input and does provide external output. Internal input is transmitted through COMMON. There is no internal output. The internal input consists of:

AVCH2D	AVCH2F	AVCH2P	AVECOD	AVECOF
AVECOP	AVECSD	AVECSF	AVECSP	AVENOD
AVENOF	AVENOP	AVET	INDIC	PHIBAR
RHOBAR	TAUBAR	XD		

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols in Subroutine PRINTS which are not included in COMMON.

Fortran Symbol	Symbol	Description	Units
AVCH2	$[\overline{CH_2}^*]$	Equilibrium concentration of unburned hydrocarbons exclusive of $C_{(s)}$ and CO at X_D.	lb/ft^3
AVECO	$[\overline{CO}^*]$	Equilibrium concentration of CO at X_D	lb/ft^3
AVECS	$[\overline{C}_s^*]$	Equilibrium concentration of $C_{(s)}$ at X_D	lb/ft^3
AVENO	$[\overline{NO}^*]$	Concentration of NO at X_D	lb/ft^3
$AVENO_2$	$[\overline{NO_2}]$	Equivalent concentration of NO_2 at X_D	lb/1000 lb fuel burned
AVETF	$\overline{T}$	Temperature at X_D	deg F
DENOM		Constant	$\frac{ft^3 - gm}{cm^3 - lb}$
IPRINT		Indicator IPRINT = 0 if intermediate zone heading is to printed IPRINT = 1	—

Fortran Symbol	Symbol	Description	Units
		if intermediate zone heading is not to be printed IPRINT = 2 if dilution zone heading is not to be printed	
RHOBA	$\bar{\rho}$	Mean density of combustion products at X_D	lb/ft^3
TTUBAR	$\bar{\tau}$	Mean residence time at X_D	msecs
XOUT	X_D	Axial position downstream in the combustor	in

Analysis Procedure

The step-by-step procedure of Subroutine PRINTS is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Convert X_D from cm to in.
2. Convert $\bar{\tau}$ from secs to msecs.
3. Convert NO, CO, $C_{(s)}$, and CH_2 concentrations from gm/cc to lb/ft^3.
4. Convert NO concentration at X_D to the equivalent NO_2 concentration.
5. Convert $\bar{\rho}$ from gm/cc to lb/ft^3.
6. Convert $\bar{T}$ from deg K to deg F.
7. If this is the primary zone, write the primary zone heading and output. Go to step 12. If it is not the primary zone, go to step 8.
8. If this is the intermediate zone and the first written output for the zone, write the heading for the intermediate zone. If not, go to step 9.
9. If this is the intermediate zone, write the output at X_D. Go to step 12. If it is not the intermediate zone, go to step 10.
10. If this is the dilution zone and the first written output in the zone, write the heading for the dilution zone. If not, go to step 11.

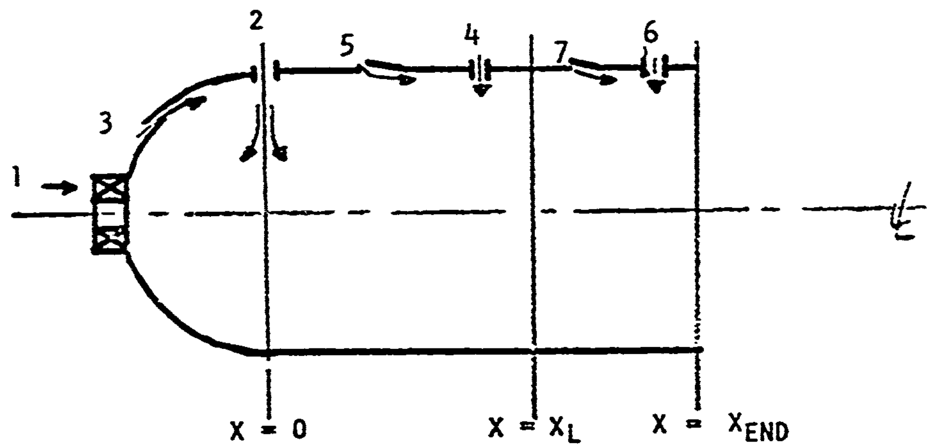
11. If this is the dilution zone, write the output for the dilution zone at X_D. Go to step 12.
12. Return.

```
      SUBROUTINE PRINTS
      REAL NO
      COMMON/OUT1/AVECSG,AVECOG,AVCH2G,AVECSP,AVECOP,AVCH2P,AVECSD,AVECO
     1D,AVCH2D,AVECSF,AVECOF,AVCH2F
      COMMON/OUT2/AVENOG,AVENOD,AVENOP,AVENOF,AVENFU,RRO,ILAST
      COMMON/OUT3/INDIC,NO(50),AVET,TAUBAR,RHOBAR,PHIBAR,IMAX,XD,
     1FBARD,XU,LEN,TAUINT,TAUDIL,VELOC
      COMMON/OUT4/CONGNO(50),DELMD(50),AREAD,ASLOPE,DMFUO,SLOPE(50),TSLO
     1PE,NOP(50),EKKD,DMFT,UDM(50),DDM(50),     FB(50),DMFUD,AIRD,DMFFED
     2,RSUBX,SIG,SIGZER,AVEMW,DMDDA(50),DMDDM(50),DMDDP(50),DMDDPP(50),F
     3PRIME(50),NOEQXD,ANO,AQQ,DIFNO(50),NOZERO(50),RDOT(50),E(50)
      NPRINT=0
      IF(INDIC.EQ.1) IPRINT=0
      XOUT=XD/2.54
      TTUBAR = TAUBAR*1000.
      DENOM=454.0*3.532E-05
      AVENO=AVENOD/DENOM
      AVECO=AVECOD/DENOM
      AVECS=AVECSD/DENOM
      AVCH2=AVCH2D/DENOM
      AVENO2 = AVENOF*46.0/30.0
      RHOBA=RHOBAR/DENOM
      AVETF=((AVET-273.16)*1.8)+32.0
      GO TO (1000,2000,3000),INDIC
 1000 CONTINUE
      WRITE(6,1010)
 1010 FORMAT(1H1)
      WRITE(6,1020)
 1020 FORMAT(48H THIS IS THE MAIN PRINTOUT FOR THE PRIMARY ZONE  /////)
      GO TO 4000
 2000 IF(IPRINT.EQ.1) GO TO 5500
      WRITE(6,1010)
      WRITE(6,2020)
 2020 FORMAT(53H THIS IS THE MAIN PRINTOUT FOR THE INTERMEDIATE ZONE
     1//////)
      IPRINT=1
      GO TO 4000
 3000 IF(IPRINT.EQ.2) GO TO 5500
      WRITE(6,1010)
      WRITE(6,3020)
 3020 FORMAT(49H THIS IS THE MAIN PRINTOUT FOR THE DILUTION ZONE /////)
      IPRINT=2
 4000 WRITE(6,5000)
 5000 FORMAT(1X,6HX(IN.),1X,3HPHI,3X,1HT,6X,3HRHO,3X,3HTAU,6X,2HNO,9X,3H
     1NO2, 9X,4HC(S), 6X,4HC(S), 8X,2HCO, 9X,2HCO, 8X,3HCH2, 8X,3HCH2 )
      WRITE(6,5100)
 5100 FORMAT(8X,4HAVE.,1X,5HDEG F,3X,4HAVE.,2X,4HAVE.,5X,3HPPM,6X,7HLBS
     1PER,7X,3HPPM,5X,7HLBS PER,7X,3HPPM,5X,7HLBS PER, 6X,3HPPM,7X,7HLBS
     2 PER)
      WRITE(6,5200)
 5200 FORMAT(19X,7HLB/CUFT,1X,4HMSEC,4X,5H(VOL),5X,7H1000 LB,6X,5H(VOL),
     14X,7H1000 LB,6X,5H(VOL),4X,7H1000 LB,5X,5H(VOL),4X,7H1000 LB)
      WRITE(6,5300)
 5300 FORMAT(43X,11HFUEL BURNED,11X,11HFUEL BURNED,11X,11HFUEL BURNED,11
     1X,11HFUEL BURNED)
 5500 WRITE(6,6000)XOUT,PHIBAR,AVETF,RHOBA,TTUBAR,AVENOP,AVENO2,AVECSP,
     1AVECSF,AVECOP,AVECOF,AVCH2P,AVCH2F
 6000 FORMAT(1X,F5.2,1X,F4.2,1X,F5.0,1X,F6.4,1X,F6.2,1X,8(E10.3,1X)//)
      IF(NPRINT.EQ.1) WRITE(6,9999)( NO(I),I=1,IMAX)
 9999 FORMAT(10X,4H  **,8E12.4)
```

```
      RETURN                                                            PRT*0600
      END                                                               PRT*0610
```

APPENDIX XVI - METHOD OF CALCULATION OF AIR DISTRIBUTION CHARACTERISTICS

Air enters the combustor liner at discrete positions over the whole length of the liner. The bulk of such flow normally enters perpendicular to the direction of the mainstream product flow and has then to be deflected and entrained before it can mix with the combustion products. This action requires a finite time (i.e., distance) to occur, and its effect upon the nitric oxide formation process has to be considered. A method has been developed, therefore, to take account of this effect. The method is consistent with the mixing assumptions made in the flow model described in this report ; it has been applied to all combustors considered in this report and is described below.



The flow behavior at each port shown in the figure above is assumed to behave as follows:

Port 1 All air entering at this position is assumed to mix with the products in the primary zone.

Port 2 Some fraction of the air, f, mixes with the primary zone and the remainder is entrained according to the law described for port 4.

Port 3 Cooling air mixes according to the relationship

$$M_X = M_3 \text{ (Distance from port 3 to X divided by distance from port 3 to } X_L)^{0.5}$$

and that part which mixes before the primary zone exit ($X = 0$), is assumed to burn in the primary zone.

Port 4 and 5 Both cooling and combustion air mix according to the relationship shown above,

$$\text{i.e., } M_X = M_4((X-X_4)/(X_L-X_4))^{0.5}$$

Port 6 and 7 This air enters the dilution zone so it is assumed that instantaneous mixing occurs (see Section 2.5).

All these independent mass flows are then summed at a particular position along the combustor to give the total airflow contained with the combustion products at that point. For example:

air burning in the primary zone M_{pz} is given by,

$$M_{pz} = M_0 = M_1 + f_{M_2} + M_{3_{x=0}}$$

air at position X $(0 < X < X_L)$

$$M_x = (1-f)\, M_2 + M_{3_x} + M_{4_x} + M_{5_x} + M_{p_z}$$

air at position X, $(X_7 < X < X_6)$

$$M_x = \sum_1^5 M_n + M_7$$

This method was applied to combustors A and B studied in this report and in each case the value of f, the fraction of air entering the primary zone from the first row of air ports, was assumed to equal one third. For Combustor A this value corresponded to the value recommended by the designers, but in the case of Combustor B, the value was estimated based on the design features. Errors in the predictions of nitric oxide emission levels from this latter estimate can be expected to be negligible as the total airflow through port 2 represents less than two per cent of the total airflow.